LAMMPS Documentation

The LAMMPS Developers

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USER DOCUMENTATION

I 3 Mar 2020 version **1**

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Part I

3 Mar 2020 version

What is a LAMMPS version?

LAMMPS stands for Large-scale Atomic/Molecular Massively Parallel Simulator.

LAMMPS is a classical molecular dynamics simulation code with a focus on materials modeling. It was designed to run efficiently on parallel computers. It was developed originally at Sandia National Laboratories, a US Department of Energy facility. The majority of funding for LAMMPS has come from the US Department of Energy (DOE). LAMMPS is an open-source code, distributed freely under the terms of the GNU Public License (GPL).

The LAMMPS website has a variety of information about the code. It includes links to an on-line version of this manual, a mailing list where users can post questions, and a GitHub site where all LAMMPS development is coordinated.

The content for this manual is part of the LAMMPS distribution. You can build a local copy of the Manual as HTML pages or a PDF file, by following the steps on the *Manual build* doc page. There is also a Developer.pdf document which gives a brief description of the basic code structure of LAMMPS.

Once you are familiar with LAMMPS, you may want to bookmark *this page* since it gives quick access to a doc page for every LAMMPS command.

CHAPTER

ONE

INTRODUCTION

These pages provide a brief introduction to LAMMPS.

1.1 Overview of LAMMPS

LAMMPS is a classical molecular dynamics (MD) code that models ensembles of particles in a liquid, solid, or gaseous state. It can model atomic, polymeric, biological, solid-state (metals, ceramics, oxides), granular, coarse-grained, or macroscopic systems using a variety of interatomic potentials (force fields) and boundary conditions. It can model 2d or 3d systems with only a few particles up to millions or billions.

LAMMPS can be built and run on a laptop or desktop machine, but is designed for parallel computers. It will run on any parallel machine that supports the MPI message-passing library. This includes shared-memory boxes and distributed-memory clusters and supercomputers.

LAMMPS is written in C++. Earlier versions were written in F77 and F90. See the History page of the website for details. All versions can be downloaded from the LAMMPS website.

LAMMPS is designed to be easy to modify or extend with new capabilities, such as new force fields, atom types, boundary conditions, or diagnostics. See the *Modify* doc page for more details.

In the most general sense, LAMMPS integrates Newton's equations of motion for a collection of interacting particles. A single particle can be an atom or molecule or electron, a coarse-grained cluster of atoms, or a mesoscopic or macroscopic clump of material. The interaction models that LAMMPS includes are mostly short-range in nature; some long-range models are included as well.

LAMMPS uses neighbor lists to keep track of nearby particles. The lists are optimized for systems with particles that are repulsive at short distances, so that the local density of particles never becomes too large. This is in contrast to methods used for modeling plasma or gravitational bodies (e.g. galaxy formation).

On parallel machines, LAMMPS uses spatial-decomposition techniques to partition the simulation domain into small sub-domains of equal computational cost, one of which is assigned to each processor. Processors communicate and store "ghost" atom information for atoms that border their sub-domain.

1.2 What does a LAMMPS version mean

The LAMMPS "version" is the date when it was released, such as 1 May 2014. LAMMPS is updated continuously. Whenever we fix a bug or add a feature, we release it in the next *patch* release, which are typically made every couple of weeks. Info on patch releases are on this website page. Every few months, the latest patch release is subjected to more thorough testing and labeled as a *stable* version.

Each version of LAMMPS contains all the features and bug-fixes up to and including its version date.

The version date is printed to the screen and logfile every time you run LAMMPS. It is also in the file src/version.h and in the LAMMPS directory name created when you unpack a tarball. And it is on the first page of the *manual*.

- If you browse the HTML doc pages on the LAMMPS WWW site, they always describe the most current patch release of LAMMPS.
- If you browse the HTML doc pages included in your tarball, they describe the version you have, which may be older.

1.3 LAMMPS features

LAMMPS is a classical molecular dynamics (MD) code with these general classes of functionality:

1. *General features*
2. *Particle and model types*
3. *Interatomic potentials (force fields)*
4. *Atom creation*
5. *Ensembles, constraints, and boundary conditions*
6. *Integrators*
7. *Diagnostics*
8. *Output*
9. *Multi-replica models*
10. *Pre- and post-processing*
11. *Specialized features (beyond MD itself)*

1.3.1 General features

- runs on a single processor or in parallel
- distributed-memory message-passing parallelism (MPI)
- spatial-decomposition of simulation domain for parallelism
- open-source distribution
- highly portable C++
- optional libraries used: MPI and single-processor FFT
- GPU (CUDA and OpenCL), Intel Xeon Phi, and OpenMP support for many code features

- easy to extend with new features and functionality
- runs from an input script
- syntax for defining and using variables and formulas
- syntax for looping over runs and breaking out of loops
- run one or multiple simulations simultaneously (in parallel) from one script
- build as library, invoke LAMMPS through library interface or provided Python wrapper
- couple with other codes: LAMMPS calls other code, other code calls LAMMPS, umbrella code calls both

1.3.2 Particle and model types

(*atom style* command)

- atoms
- coarse-grained particles (e.g. bead-spring polymers)
- united-atom polymers or organic molecules
- all-atom polymers, organic molecules, proteins, DNA
- metals
- granular materials
- coarse-grained mesoscale models
- finite-size spherical and ellipsoidal particles
- finite-size line segment (2d) and triangle (3d) particles
- point dipole particles
- rigid collections of particles
- hybrid combinations of these

1.3.3 Interatomic potentials (force fields)

(*pair style*, *bond style*, *angle style*, *dihedral style*, *improper style*, *kspace style* commands)

- pairwise potentials: Lennard-Jones, Buckingham, Morse, Born-Mayer-Huggins, Yukawa, soft, class 2 (COMPASS), hydrogen bond, tabulated
- charged pairwise potentials: Coulombic, point-dipole
- many-body potentials: EAM, Finnis/Sinclair EAM, modified EAM (MEAM), embedded ion method (EIM), EDIP, ADP, Stillinger-Weber, Tersoff, REBO, AIREBO, ReaxFF, COMB, SNAP, Streitz-Mintmire, 3-body polymorphic
- long-range interactions for charge, point-dipoles, and LJ dispersion: Ewald, Wolf, PPPM (similar to particle-mesh Ewald)
- polarization models: *QEq*, *core/shell model*, *Drude dipole model*
- charge equilibration (QEq via dynamic, point, shielded, Slater methods)
- coarse-grained potentials: DPD, GayBerne, REsquared, colloidal, DLVO
- mesoscopic potentials: granular, Peridynamics, SPH

- electron force field (eFF, AWPMD)
- bond potentials: harmonic, FENE, Morse, nonlinear, class 2, quartic (breakable)
- angle potentials: harmonic, CHARMM, cosine, cosine/squared, cosine/periodic, class 2 (COMPASS)
- dihedral potentials: harmonic, CHARMM, multi-harmonic, helix, class 2 (COMPASS), OPLS
- improper potentials: harmonic, cvff, umbrella, class 2 (COMPASS)
- polymer potentials: all-atom, united-atom, bead-spring, breakable
- water potentials: TIP3P, TIP4P, SPC
- implicit solvent potentials: hydrodynamic lubrication, Debye
- force-field compatibility with common CHARMM, AMBER, DREIDING, OPLS, GROMACS, COMPASS options
- access to the OpenKIM Repository of potentials via *kim_init, kim_interactions, and kim_query* commands
- hybrid potentials: multiple pair, bond, angle, dihedral, improper potentials can be used in one simulation
- overlaid potentials: superposition of multiple pair potentials

1.3.4 Atom creation

(*read_data*, *lattice*, *create_atoms*, *delete_atoms*, *displace_atoms*, *replicate* commands)

- read in atom coords from files
- create atoms on one or more lattices (e.g. grain boundaries)
- delete geometric or logical groups of atoms (e.g. voids)
- replicate existing atoms multiple times
- displace atoms

1.3.5 Ensembles, constraints, and boundary conditions

(*fix* command)

- 2d or 3d systems
- orthogonal or non-orthogonal (triclinic symmetry) simulation domains
- constant NVE, NVT, NPT, NPH, Parrinello/Rahman integrators
- thermostatting options for groups and geometric regions of atoms
- pressure control via Nose/Hoover or Berendsen barostatting in 1 to 3 dimensions
- simulation box deformation (tensile and shear)
- harmonic (umbrella) constraint forces
- rigid body constraints
- SHAKE bond and angle constraints
- Monte Carlo bond breaking, formation, swapping
- atom/molecule insertion and deletion
- walls of various kinds

- non-equilibrium molecular dynamics (NEMD)
- variety of additional boundary conditions and constraints

1.3.6 Integrators

(*run*, *run_style*, *minimize* commands)

- velocity-Verlet integrator
- Brownian dynamics
- rigid body integration
- energy minimization via conjugate gradient or steepest descent relaxation
- rRESPA hierarchical timestepping
- rerun command for post-processing of dump files

1.3.7 Diagnostics

- see various flavors of the *fix* and *compute* commands

1.3.8 Output

(*dump*, *restart* commands)

- log file of thermodynamic info
- text dump files of atom coords, velocities, other per-atom quantities
- binary restart files
- parallel I/O of dump and restart files
- per-atom quantities (energy, stress, centro-symmetry parameter, CNA, etc)
- user-defined system-wide (log file) or per-atom (dump file) calculations
- spatial and time averaging of per-atom quantities
- time averaging of system-wide quantities
- atom snapshots in native, XYZ, XTC, DCD, CFG formats

1.3.9 Multi-replica models

- *nudged elastic band*
- *parallel replica dynamics*
- *temperature accelerated dynamics*
- *parallel tempering*

1.3.10 Pre- and post-processing

- A handful of pre- and post-processing tools are packaged with LAMMPS, some of which can convert input and output files to/from formats used by other codes; see the *Toos* doc page.
- Our group has also written and released a separate toolkit called Pizza.py which provides tools for doing setup, analysis, plotting, and visualization for LAMMPS simulations. Pizza.py is written in Python and is available for download from the Pizza.py WWW site.

1.3.11 Specialized features

LAMMPS can be built with optional packages which implement a variety of additional capabilities. See the *Packages* doc page for details.

These are LAMMPS capabilities which you may not think of as typical classical MD options:

- *static* and *dynamic load-balancing*
- *generalized aspherical particles*
- *stochastic rotation dynamics (SRD)*
- *real-time visualization and interactive MD*
- calculate *virtual diffraction patterns*
- *atom-to-continuum coupling* with finite elements
- coupled rigid body integration via the *POEMS* library
- *QM/MM coupling*
- Monte Carlo via *GCMC* and *tfMC* and *atom swapping*
- *path-integral molecular dynamics (PIMD)* and *this as well*
- *Direct Simulation Monte Carlo* for low-density fluids
- *Peridynamics mesoscale modeling*
- *Lattice Boltzmann fluid*
- *targeted* and *steered* molecular dynamics
- *two-temperature electron model*

1.4 LAMMPS non-features

LAMMPS is designed to be a fast, parallel engine for molecular dynamics (MD) simulations. It provides only a modest amount of functionality for setting up simulations and analyzing their output.

Specifically, LAMMPS was not conceived and designed for:

- being run through a GUI
- building molecular systems, or building molecular topologies
- assign force-field coefficients automagically
- perform sophisticated analysis of your MD simulation
- visualize your MD simulation interactively

- plot your output data

Over the years some of these limitations have been reduced or removed, through features added to LAMMPS or external tools that either closely interface with LAMMPS or extend LAMMPS.

Here are suggestions on how to perform these tasks:

- **GUI:** LAMMPS can be built as a library and a Python wrapper that wraps the library interface is provided. Thus, GUI interfaces can be written in Python (or C or C++ if desired) that run LAMMPS and visualize or plot its output. Examples of this are provided in the python directory and described on the *Python* doc page. Also, there are several external wrappers or GUI front ends.
- **Builder:** Several pre-processing tools are packaged with LAMMPS. Some of them convert input files in formats produced by other MD codes such as CHARMM, AMBER, or Insight into LAMMPS input formats. Some of them are simple programs that will build simple molecular systems, such as linear bead-spring polymer chains. The moltemplate program is a true molecular builder that will generate complex molecular models. See the *Tools* doc page for details on tools packaged with LAMMPS. The Pre/post processing page of the LAMMPS website describes a variety of 3rd party tools for this task. Furthermore, some LAMMPS internal commands allow to reconstruct, or selectively add topology information, as well as provide the option to insert molecule templates instead of atoms for building bulk molecular systems.
- **Force-field assignment:** The conversion tools described in the previous bullet for CHARMM, AMBER, and Insight will also assign force field coefficients in the LAMMPS format, assuming you provide CHARMM, AMBER, or BIOVIA (formerly Accelrys) force field files. The tools ParmEd and InterMol are particularly powerful and flexible in converting force field and topology data between various MD simulation programs.
- **Simulation analysis:** If you want to perform analysis on-the-fly as your simulation runs, see the *compute* and *fix* doc pages, which list commands that can be used in a LAMMPS input script. Also see the *Modify* doc page for info on how to add your own analysis code or algorithms to LAMMPS. For post-processing, LAMMPS output such as *dump file snapshots* can be converted into formats used by other MD or post-processing codes. To some degree, that conversion can be done directly inside of LAMMPS by interfacing to the VMD molfile plugins. The *rerun* command also allows to do some post-processing of existing trajectories, and through being able to read a variety of file formats, this can also be used for analyzing trajectories from other MD codes. Some post-processing tools packaged with LAMMPS will do these conversions. Scripts provided in the tools/python directory can extract and massage data in dump files to make it easier to import into other programs. See the *Tools* doc page for details on these various options.
- **Visualization:** LAMMPS can produce NETPBM, JPG or PNG snapshot images on-the-fly via its *dump image* command and pass them to an external program, FFmpeg to generate movies from them. For high-quality, interactive visualization there are many excellent and free tools available. See the Other Codes page page of the LAMMPS website for visualization packages that can use LAMMPS output data.
- **Plotting:** See the next bullet about Pizza.py as well as the *Python* doc page for examples of plotting LAMMPS output. Scripts provided with the *python* tool in the tools directory will extract and massage data in log and dump files to make it easier to analyze and plot. See the *Tools* doc page for more discussion of the various tools.
- **Pizza.py:** Our group has also written a separate toolkit called Pizza.py which can do certain kinds of setup, analysis, plotting, and visualization (via OpenGL) for LAMMPS simulations. It thus provides some functionality for several of the above bullets. Pizza.py is written in Python and is available for download from this page.

1.5 LAMMPS open-source license

LAMMPS is a freely-available open-source code, distributed under the terms of the GNU Public License, which means you can use or modify the code however you wish.

LAMMPS comes with no warranty of any kind. As each source file states in its header, it is a copyrighted code that is distributed free-of- charge, under the terms of the GNU Public License (GPL). This is often referred to as open-source distribution - see www.gnu.org or www.opensource.org. The legal text of the GPL is in the LICENSE file included in the LAMMPS distribution.

Here is a summary of what the GPL means for LAMMPS users:

(1) Anyone is free to use, modify, or extend LAMMPS in any way they choose, including for commercial purposes.

(2) If you distribute a modified version of LAMMPS, it must remain open-source, meaning you distribute it under the terms of the GPL. You should clearly annotate such a code as a derivative version of LAMMPS.

(3) If you release any code that includes LAMMPS source code, then it must also be open-sourced, meaning you distribute it under the terms of the GPL.

(4) If you give LAMMPS files to someone else, the GPL LICENSE file and source file headers (including the copyright and GPL notices) should remain part of the code.

1.6 Authors of LAMMPS

The primary LAMMPS developers are at Sandia National Labs and Temple University:

- Steve Plimpton, sjplimp at sandia.gov
- Aidan Thompson, athomps at sandia.gov
- Stan Moore, stamoor at sandia.gov
- Axel Kohlmeyer, akohlmey at gmail.com
- Richard Berger, richard.berger at temple.edu

Past developers include Paul Crozier and Mark Stevens, both at Sandia, and Ray Shan, now at Materials Design.

The Authors page of the LAMMPS website has a comprehensive list of all the individuals who have contributed code for a new feature or command or tool to LAMMPS.

The following folks deserve special recognition. Many of the packages they have written are unique for an MD code and LAMMPS would not be as general-purpose as it is without their expertise and efforts.

- Metin Aktulga (MSU), USER-REAXC package for C version of ReaxFF
- Mike Brown (Intel), GPU and USER-INTEL packages
- Colin Denniston (U Western Ontario), USER-LB package
- Georg Ganzenmuller (EMI), USER-SMD and USER-SPH packages
- Andres Jaramillo-Botero (Caltech), USER-EFF package for electron force field
- Reese Jones (Sandia) and colleagues, USER-ATC package for atom/continuum coupling
- Christoph Kloss (DCS Computing), LIGGGHTS code for granular materials, built on top of LAMMPS
- Rudra Mukherjee (JPL), POEMS package for articulated rigid body motion

- Trung Ngyuen (Northwestern U), GPU and RIGID and BODY packages
- Mike Parks (Sandia), PERI package for Peridynamics
- Roy Pollock (LLNL), Ewald and PPPM solvers
- Christian Trott (Sandia), USER-CUDA and KOKKOS packages
- Ilya Valuev (JIHT), USER-AWPMD package for wave packet MD
- Greg Wagner (Northwestern U), MEAM package for MEAM potential

---

As discussed on the History page of the website, LAMMPS originated as a cooperative project between DOE labs and industrial partners. Folks involved in the design and testing of the original version of LAMMPS were the following:

- John Carpenter (Mayo Clinic, formerly at Cray Research)
- Terry Stouch (Lexicon Pharmaceuticals, formerly at Bristol Myers Squibb)
- Steve Lustig (Dupont)
- Jim Belak and Roy Pollock (LLNL)

1.7 Additional website links

The LAMMPS website has a variety of additional info about LAMMPS, beyond what is in this manual. Some of the other pages in this Intr are included in this list.

- Brief intro and recently added significant features
- List of features
- List of non-features
- Recent bug fixes and new features
- Download info
- GitHub site
- SourceForge site
- LAMMPS open-source license
- Glossary of MD terms relevant to LAMMPS
- LAMMPS highlights with images
- LAMMPS highlights with movies
- Mail list
- Workshops
- Tutorials
- Developer guide
- Pre- and post-processing tools for LAMMPS
- Other software usable with LAMMPS
- Viz tools usable with LAMMPS
- Benchmark performance

- Publications that have cited LAMMPS
- Authors of LAMMPS
- History of LAMMPS development
- Funding for LAMMPS

CHAPTER

TWO

INSTALL LAMMPS

You can download LAMMPS as an executable or as source code.

With source code, you also have to *build LAMMPS*. But you have more flexibility as to what features to include or exclude in the build. If you plan to *modify or extend LAMMPS*, then you need the source code.

2.1 Download an executable for Linux

Binaries are available for different versions of Linux:

Pre-built Ubuntu Linux executables
Pre-built Fedora Linux executables
Pre-built EPEL Linux executables (RHEL, CentOS)
Pre-built OpenSuse Linux executables
Gentoo Linux executable
Arch Linux build-script

2.1.1 Pre-built Ubuntu Linux executables

A pre-built LAMMPS executable suitable for running on the latest Ubuntu Linux versions, can be downloaded as a Debian package. This allows you to install LAMMPS with a single command, and stay up-to-date with the current version of LAMMPS by simply updating your operating system.

To install the appropriate personal-package archive (PPA), do the following once:

```
$ sudo add-apt-repository ppa:gladky-anton/lammps
$ sudo apt-get update
```

To install LAMMPS do the following once:

```
$ sudo apt-get install lammps-daily
```

This downloads an executable named "lmp_daily" to your box, which can then be used in the usual way to run input scripts:

```
$ lmp_daily -in in.lj
```

To update LAMMPS to the most current version, do the following:

```
$ sudo apt-get update
```

which will also update other packages on your system.

To get a copy of the current documentation and examples:

```
$ sudo apt-get install lammps-daily-doc
```

which will download the doc files in /usr/share/doc/lammps-daily-doc/doc and example problems in /usr/share/doc/lammps-doc/examples.

Note that you may still wish to download the tarball to get potential files and auxiliary tools.

To un-install LAMMPS, do the following:

```
$ sudo apt-get remove lammps-daily
```

Note that the lammps-daily executable is built with the following sequence of make commands, as if you had done the same with the unpacked tarball files in the src directory:

```
$ make yes-all
$ make no-lib
$ make mpi
```

Thus it builds with FFTW3 and OpenMPI.

Thanks to Anton Gladky (gladky.anton at gmail.com) for setting up this Ubuntu package capability.

2.1.2 Pre-built Fedora Linux executables

Pre-built LAMMPS packages for stable releases are available in the Fedora Linux distribution as of version 28. The packages can be installed via the dnf package manager. There are 3 basic varieties (lammps = no MPI, lammps-mpich = MPICH MPI library, lammps-openmpi = OpenMPI MPI library) and for each support for linking to the C library interface (lammps-devel, lammps-mpich-devel, lammps-openmpi-devel), the header for compiling programs using the C library interface (lammps-headers), and the LAMMPS python module for Python 3. All packages can be installed at the same time and the name of the LAMMPS executable is *lmp* and *lmp_openmpi* or *lmp_mpich* respectively. By default, *lmp* will refer to the serial executable, unless one of the MPI environment modules is loaded ("module load mpi/mpich-x86_64" or "module load mpi/openmpi-x86_64"). Then the corresponding parallel LAMMPS executable can be used. The same mechanism applies when loading the LAMMPS python module.

To install LAMMPS with OpenMPI and run an input in.lj with 2 CPUs do:

```
$ dnf install lammps-openmpi
$ module load mpi/openmpi-x86_64
$ mpirun -np 2 lmp -in in.lj
```

The "dnf install" command is needed only once. In case of a new LAMMPS stable release, "dnf update" will automatically update to the newer version as soon at the RPM files are built and uploaded to the download mirrors. The "module load" command is needed once per (shell) session or shell terminal instance, unless it is automatically loaded from the shell profile.

The LAMMPS binary is built with the *KIM package* which results in the above command also installing the *kim-api* binaries when LAMMPS is installed. In order to use potentials from openkim.org, you can install the *openkim-models* package

```
$ dnf install openkim-models
```

Please use "lmp -help" to see which compilation options, packages, and styles are included in the binary.

Thanks to Christoph Junghans (LANL) for making LAMMPS available in Fedora.

2.1.3 Pre-built EPEL Linux executable

Pre-built LAMMPS (and KIM) packages for stable releases are available in the Extra Packages for Enterprise Linux (EPEL) repository for use with Red Hat Enterprise Linux (RHEL) or CentOS version 7.x and compatible Linux distributions. Names of packages, executable, and content are the same as described above for Fedora Linux. But RHEL/CentOS 7.x uses the "yum" package manager instead of "dnf" in Fedora 28.

Please use "lmp -help" to see which compilation options, packages, and styles are included in the binary.

Thanks to Christoph Junghans (LANL) for making LAMMPS available in EPEL.

2.1.4 Pre-built OpenSuse Linux executable

A pre-built LAMMPS package for stable releases is available in OpenSuse as of Leap 15.0. You can install the package with:

```
$ zypper install lammps
```

This includes support for OpenMPI. The name of the LAMMPS executable is *lmp*. Thus to run an input in parallel on 2 CPUs you would do:

```
$ mpirun -np 2 lmp -in in.lj
```

Please use "lmp -help" to see which compilation options, packages, and styles are included in the binary.

The LAMMPS binary is built with the *KIM package* which results in the above command also installing the *kim-api* binaries when LAMMPS is installed. In order to use potentials from openkim.org, you can install the *openkim-models* package

```
$ zypper install openkim-models
```

Thanks to Christoph Junghans (LANL) for making LAMMPS available in OpenSuse.

2.1.5 Gentoo Linux executable

LAMMPS is part of Gentoo's main package tree and can be installed by typing:

```
% emerge --ask lammps
```

Note that in Gentoo the LAMMPS source is downloaded and the package is built on the your machine.

Certain LAMMPS packages can be enable via USE flags, type

```
% equery uses lammps
```

for details.

Thanks to Nicolas Bock and Christoph Junghans (LANL) for setting up this Gentoo capability.

2.1.6 Archlinux build-script

LAMMPS is available via Arch's unofficial Arch User repository (AUR). There are three scripts available, named lammps, lammps-beta and lammps-git. They respectively package the stable, patch and git releases.

To install, you will need to have the git package installed. You may use any of the above names in-place of lammps.

```
$ git clone https://aur.archlinux.org/lammps.git
$ cd lammps
$ makepkg -s
$ makepkg -i
```

To update, you may repeat the above, or change into the cloned directory, and execute the following, after which, if there are any changes, you may use makepkg as above.

```
$ git pull
```

Alternatively, you may use an AUR helper to install these packages.

Note that the AUR provides build-scripts that download the source and the build the package on your machine.

2.2 Download an executable for Mac

LAMMPS can be downloaded, built, and configured for OS X on a Mac with Homebrew. (Alternatively, see the install instructions for *Download an executable via Conda*.) The following LAMMPS packages are unavailable at this time because of additional needs not yet met: GPU, KOKKOS, LATTE, MSCG, MESSAGE, MPIIO POEMS VORONOI.

After installing Homebrew, you can install LAMMPS on your system with the following commands:

```
% brew install lammps
```

This will install the executables "lammps_serial" and "lammps_mpi", as well as the LAMMPS "doc", "potentials", "tools", "bench", and "examples" directories.

Once LAMMPS is installed, you can test the installation with the Lennard-Jones benchmark file:

```
% brew test lammps -v
```

The LAMMPS binary is built with the *KIM package* which results in Homebrew also installing the *kim-api* binaries when LAMMPS is installed. In order to use potentials from openkim.org, you can install the *openkim-models* package

```
% brew install openkim-models
```

If you have problems with the installation you can post issues to this link.

Thanks to Derek Thomas (derekt at cello.t.u-tokyo.ac.jp) for setting up the Homebrew capability.

2.3 Download an executable for Windows

Pre-compiled Windows installers which install LAMMPS executables on a Windows system can be downloaded from this site:

http://packages.lammps.org/windows.html

Note that each installer package has a date in its name, which corresponds to the LAMMPS version of the same date. Installers for current and older versions of LAMMPS are available. 32-bit and 64-bit installers are available, and each installer contains both a serial and parallel executable. The installer site also explains how to install the Windows MPI package (MPICH2 from Argonne National Labs), needed to run in parallel.

The LAMMPS binaries contain all optional packages included in the source distribution except: KIM, KOKKOS, USER-INTEL, and USER-QMMM. The serial version also does not include the MPIIO and USER-LB packages. GPU support is provided for OpenCL.

The installer site also has instructions on how to run LAMMPS under Windows, once it is installed, in both serial and parallel.

When you download the installer package, you run it on your Windows machine. It will then prompt you with a dialog, where you can choose the installation directory, unpack and copy several executables, potential files, documentation pdfs, selected example files, etc. It will then update a few system settings (e.g. PATH, LAMMPS_POTENTIALS) and add an entry into the Start Menu (with references to the documentation, LAMMPS homepage and more). From that menu, there is also a link to an uninstaller that removes the files and undoes the environment manipulations.

Note that to update to a newer version of LAMMPS, you should typically uninstall the version you currently have, download a new installer, and go through the install procedure described above. I.e. the same procedure for installing/updating most Windows programs. You can install multiple versions of LAMMPS (in different directories), but only the executable for the last-installed package will be found automatically, so this should only be done for debugging purposes.

Thanks to Axel Kohlmeyer (Temple U, akohlmey at gmail.com) for setting up this Windows capability.

2.4 Download an executable for Linux or Mac via Conda

Binaries are available for macOS or Linux via Conda.

First, one must setup the Conda package manager on your system. Follow the instructions to install Miniconda, then create a conda environment (named *my-lammps-env* or whatever you prefer) for your lammps install:

```
% conda config --add channels conda-forge
% conda create -n my-lammps-env
```

Then, you can install lammps on your system with the following command:

```
% conda activate my-lammps-env
% conda install lammps
```

The LAMMPS binary is built with the *KIM package* which results in Conda also installing the *kim-api* binaries when LAMMPS is installed. In order to use potentials from openkim.org, you can install the *openkim-models* package

```
% conda install openkim-models
```

If you have problems with the installation you can post issues to this link. Thanks to Jan Janssen (Max-Planck-Institut fuer Eisenforschung) for setting up the Conda capability.

2.5 Download source and documentation as a tarball

You can download a current LAMMPS tarball from the download page of the LAMMPS website.

You have two choices of tarballs, either the most recent stable release or the most current patch release. Stable releases occur a few times per year, and undergo more testing before release. Patch releases occur a couple times per month. The new contents in all releases are listed on the bug and feature page of the website.

Both tarballs include LAMMPS documentation (HTML and PDF files) corresponding to that version. The download page also has an option to download the current-version LAMMPS documentation by itself.

Older versions of LAMMPS can also be downloaded from this page.

Once you have a tarball, unzip and untar it with the following command:

```
$ tar -xzvf lammps\*.tar.gz
```

This will create a LAMMPS directory with the version date in its name, e.g. lammps-23Jun18.

You can also download a zip file via the "Clone or download" button on the LAMMPS GitHub site. The file name will be lammps-master.zip which can be unzipped with the following command, to create a lammps-master dir:

```
$ unzip lammps\*.zip
```

This version is the most up-to-date LAMMPS development version. It will have the date of the most recent patch release (see the file src/version.h). But it will also include any new bug-fixes or features added since the last patch release. They will be included in the next patch release tarball.

If you download a current LAMMPS tarball, one way to stay current as new patch tarballs are released, is to download a patch file which you can apply to your local directory to update it for each new patch release. (Or of course you could just download the newest tarball periodically.)

The patch files are posted on the bug and feature page of the website, along with a list of changed files and details about what is in the new patch release. Instructions for applying a patch file are on the *Install patch* doc page.

2.6 Download the LAMMPS source with git

All LAMMPS development is coordinated through the "LAMMPS GitHub site". If you clone the LAMMPS repository onto your local machine, it has several advantages:

- You can stay current with changes to LAMMPS with a single git command.
- You can create your own development branches to add code to LAMMPS.
- You can submit your new features back to GitHub for inclusion in LAMMPS.

You must have git installed on your system to use the commands explained below to communicate with the git servers on GitHub. For people still using subversion (svn), GitHub also provides limited support for subversion clients.

Warning: As of October 2016, the official home of public LAMMPS development is on GitHub. The previously advertised LAMMPS git repositories on git.lammps.org and bitbucket.org are now deprecated or offline.

You can follow LAMMPS development on 3 different git branches:

- **stable** : this branch is updated with every stable release
- **unstable** : this branch is updated with every patch release
- **master** : this branch continuously follows ongoing development

To access the git repositories on your box, use the clone command to create a local copy of the LAMMPS repository with a command like:

```
$ git clone -b unstable https://github.com/lammps/lammps.git mylammps
```

where "mylammps" is the name of the directory you wish to create on your machine and "unstable" is one of the 3 branches listed above. (Note that you actually download all 3 branches; you can switch between them at any time using "git checkout <branch name>".)

Once the command completes, your directory will contain the same files as if you unpacked a current LAMMPS tarball, with the exception, that the HTML documentation files are not included. They can be fetched from the LAMMPS website by typing "make fetch" in the doc directory. Or they can be generated from the content provided in doc/src by typing "make html" from the doc directory.

After initial cloning, as bug fixes and new features are added to LAMMPS, as listed on *this page*, you can stay up-to-date by typing the following git commands from within the "mylammps" directory:

```
$ git checkout unstable      # not needed if you always stay in this branch
$ git checkout stable        # use one of the 3 checkout commands
$ git checkout master
$ git pull
```

Doing a "pull" will not change any files you have added to the LAMMPS directory structure. It will also not change any existing LAMMPS files you have edited, unless those files have changed in the repository. In that case, git will attempt to merge the new repository file with your version of the file and tell you if there are any conflicts. See the git documentation for details.

If you want to access a particular previous release version of LAMMPS, you can instead "checkout" any version with a published tag. See the output of "git tag -l" for the list of tags. The git command to do this is as follows.

```
$ git checkout tagID
```

Stable versions and what tagID to use for a particular stable version are discussed on *this page*. Note that this command will print some warnings, because in order to get back to the latest revision and to be able to update with "git pull" again, you first will need to first type "git checkout unstable" (or check out any other desired branch).

Once you have updated your local files with a "git pull" (or "git checkout"), you still need to re-build LAMMPS if any source files have changed. To do this, you should cd to the src directory and type:

```
$ make purge             # remove any deprecated src files
$ make package-update    # sync package files with src files
$ make foo               # re-build for your machine (mpi, serial, etc)
```

just as described on the *Install patch* doc page, after a patch has been installed.

Warning: If you wish to edit/change a src file that is from a package, you should edit the version of the file inside the package sub-directory with src, then re-install the package. The version in the source directory is merely a copy and will be wiped out if you type "make package-update".

Warning: The GitHub servers support both the "git://" and "https://" access protocols for anonymous read-only access. If you have a correspondingly configured GitHub account, you may also use SSH access with the URL "git@github.com:lammps/lammps.git".

The LAMMPS GitHub project is managed by Christoph Junghans (LANL, junghans at lanl.gov), Axel Kohlmeyer (Temple U, akohlmey at gmail.com) and Richard Berger (Temple U, richard.berger at temple.edu).

2.7 Applying patches

It is easy to stay current with the most recent LAMMPS patch releases if you use git to track the LAMMPS development. Instructions for how to stay current are on the *Download the LAMMPS source with git* page.

If you prefer to download a tarball, as described on the *Install git* doc page, you can stay current by downloading "patch files" when new patch releases are made. A link to a patch file is posted on the bug and feature page of the LAMMPS website, along with a list of changed files and details about what is in the new patch release. This page explains how to apply the patch file to your local LAMMPS directory.

Note: You should not apply patch files to a local git checkout of LAMMPS, only to an unpacked tarball. Use git commands to update such a version of the LAMMPS source code.

Here are the steps to apply a patch file. Note that if your version of LAMMPS is several patch releases behind, you need to apply all the intervening patch files in succession to bring your version of LAMMPS up to date.

- Download the patch file. You may have to shift-click in your browser to download the file instead of display it. Patch files have names like patch.12Dec16.
- Put the patch file in your top-level LAMMPS directory, where the LICENSE and README files are.
- Apply the patch by typing the following command from your top-level LAMMPS directory, where the redirected file is the name of the patch file.

```
$ patch -bp1 < patch.12Dec16
```

- A list of updated files print out to the screen. The -b switch creates backup files of your originals (e.g. src/force.cpp.orig), so you can manually undo the patch if something goes wrong.
- Type the following from the src directory, to enforce consistency between the src and package directories. This is OK to do even if you don't use one or more packages. If you are applying several patches successively, you only need to type this once at the end. The purge command removes deprecated src files if any were removed by the patch from package sub-directories.

```
$ make purge
$ make package-update
```

- Re-build LAMMPS via the "make" command.

Warning: If you wish to edit/change a source file that is part of a package, you should edit the version of the file inside the package folder in src, and then re-install or update the package. The version in the src directory is merely a copy and will be wiped out when you type "make package-update".

These are the files and sub-directories in the LAMMPS distribution:

README	text file
LICENSE	GNU General Public License (GPL)
bench	benchmark problems
cmake	CMake build files
doc	documentation
examples	simple test problems
lib	additional provided or external libraries
potentials	interatomic potential files
python	Python wrapper on LAMMPS
src	source files
tools	pre- and post-processing tools

You will have all of these if you download source. You will only have some of them if you download executables, as explained on the pages listed above.

CHAPTER

THREE

BUILD LAMMPS

LAMMPS can be built as an executable or library from source code via either traditional makefiles (which may require manual editing) for use with GNU make or gmake, or a build environment generated by CMake (Unix Makefiles, Xcode, Visual Studio, KDevelop or more). As an alternative you can download a package with pre-built executables as described on the *Install* doc page.

3.1 Build LAMMPS with CMake

This page is a short summary of how to use CMake to build LAMMPS. Details on CMake variables that enable specific LAMMPS build options are given on the pages linked to from the *Build* doc page.

Richard Berger (Temple U) has also written a more comprehensive guide for how to use CMake to build LAMMPS. If you are new to CMake it is a good place to start.

Building LAMMPS with CMake is a two-step process. First you use CMake to create a build environment in a new directory. On Linux systems, this will be based on makefiles for use with make. Then you use the make command to build LAMMPS, which uses the created Makefile(s). Example:

```
cd lammps                          # change to the LAMMPS distribution directory
mkdir build; cd build              # create a new directory (folder) for build
cmake [options ...] ../cmake       # configuration with (command-line) cmake
make                               # compilation
```

The cmake command will detect available features, enable selected packages and options, and will generate the build environment. By default this build environment will be created for "Unix Makefiles" on most platforms and particularly on Linux. However, alternate build tools (e.g. Ninja) and support files for Integrated Development Environments (IDE) like Eclipse, CodeBlocks, or Kate can be generated, too. This is selected via the "-G" command line flag. For the rest of the documentation we will assume that the build environment is generated for makefiles and thus the make command will be used to compile and link LAMMPS as indicated above, producing (by default) an executable called "lmp" and a library called "liblammps.a" in the "build" folder. When generating a build environment for the "Ninja" build tool, the build command would be "ninja" instead of "make".

If your machine has multiple CPU cores (most do these days), using a command like "make -jN" (with N being the number of available local CPU cores) can be much faster. If you plan to do development on LAMMPS or need to re-compile LAMMPS repeatedly, installation of the ccache (= Compiler Cache) software may speed up repeated compilation even more.

After compilation, you may optionally install the LAMMPS executable into your system with:

```
make install    # optional, copy LAMMPS executable & library elsewhere
```

This will install the lammps executable and library (if requested), some tools (if configured) and additional files like library API headers, manpages, potential and force field files. The location of the installation tree is set by the CMake variable "CMAKE_INSTALL_PREFIX" which defaults to ${HOME}/.local

---

There are 3 variants of CMake: a command-line version (cmake), a text mode UI version (ccmake), and a graphical GUI version (cmake-GUI). You can use any of them interchangeably to configure and create the LAMMPS build environment. On Linux all the versions produce a Makefile as their output. See more details on each below.

You can specify a variety of options with any of the 3 versions, which affect how the build is performed and what is included in the LAMMPS executable. Links to pages explaining all the options are listed on the *Build* doc page.

You must perform the CMake build system generation and compilation in a new directory you create. It can be anywhere on your local machine. In these Build pages we assume that you are building in a directory called "lammps/build". You can perform separate builds independently with different options, so long as you perform each of them in a separate directory you create. All the auxiliary files created by one build process (executable, object files, log files, etc) are stored in this directory or sub-directories within it that CMake creates.

Note: To perform a CMake build, no packages can be installed or a build been previously attempted in the LAMMPS src directory by using "make" commands to *perform a conventional LAMMPS build*. CMake detects if this is the case and generates an error, telling you to type "make no-all purge" in the src directory to un-install all packages. The purge removes all the *.h files auto-generated by make.

You must have CMake version 2.8 or later on your system to build LAMMPS. A handful of LAMMPS packages (KOKKOS, LATTE, MSCG) require a later version. CMake will print a message telling you if a later version is required. Installation instructions for CMake are below.

After the initial build, if you edit LAMMPS source files, or add your own new files to the source directory, you can just re-type make from your build directory and it will re-compile only the files that have changed. If you want to change CMake options you can run cmake (or ccmake or cmake-gui) again from the same build directory and alter various options; see details below. Or you can remove the entire build folder, recreate the directory and start over.

Command-line version of CMake:

```
cmake [options ...] /path/to/lammps/cmake  # build from any dir
cmake [options ...] ../cmake               # build from lammps/build
```

The cmake command takes one required argument, which is the LAMMPS cmake directory which contains the CMakeLists.txt file.

The argument can be preceeded or followed by various CMake command-line options. Several useful ones are:

```
-D CMAKE_INSTALL_PREFIX=path  # where to install LAMMPS executable/lib if desired
-D CMAKE_BUILD_TYPE=type      # type = RelWithDebInfo (default), Release, MinSizeRel,␣
↪or Debug
-G output                     # style of output CMake generates
-DVARIABLE=value              # setting for a LAMMPS feature to enable
-D VARIABLE=value             # ditto, but cannot come after CMakeLists.txt dir
-C path/to/preset/file        # load some CMake settings before configuring
```

All the LAMMPS-specific -D variables that a LAMMPS build supports are described on the pages linked to from the *Build* doc page. All of these variable names are upper-case and their values are lower-case, e.g. -D LAMMPS_SIZES=smallbig. For boolean values, any of these forms can be used: yes/no, on/off, 1/0.

On Unix/Linux machines, CMake generates a Makefile by default to perform the LAMMPS build. Alternate forms of build info can be generated via the -G switch, e.g. Visual Studio on a Windows machine, Xcode on MacOS, or KDevelop on Linux. Type "cmake –help" to see the "Generator" styles of output your system supports.

Note: When CMake runs, it prints configuration info to the screen. You should review this to verify all the features you requested were enabled, including packages. You can also see what compilers and compile options will be used for the build. Any errors in CMake variable syntax will also be flagged, e.g. mis-typed variable names or variable values.

CMake creates a CMakeCache.txt file when it runs. This stores all the settings, so that when running CMake again you can use the current folder '.' instead of the path to the LAMMPS cmake folder as the required argument to the CMake command. Either way the existing settings will be inherited unless the CMakeCache.txt file is removed.

If you later want to change a setting you can rerun cmake in the build directory with different setting. Please note that some automatically detected variables will not change their value when you rerun cmake. In these cases it is usually better to first remove all the files/directories in the build directory, or start with a fresh build directory.

Curses version (terminal-style menu) of CMake:

```
ccmake ../cmake
```

You initiate the configuration and build environment generation steps separately. For the first you have to type **c**, for the second you have to type **g**. You may need to type **c** multiple times, and may be required to edit some of the entries of CMake configuration variables in between. Please see the ccmake manual for more information.

GUI version of CMake:

```
cmake-gui ../cmake
```

You initiate the configuration and build environment generation steps separately. For the first you have to click on the **Configure** button, for the second you have to click on the **Generate** button. You may need to click on **Configure** multiple times, and may be required to edit some of the entries of CMake configuration variables in between. Please see the cmake-gui manual for more information.

Installing CMake

Check if your machine already has CMake installed:

```
which cmake             # do you have it?
which cmake3            # version 3 may have this name
cmake --version         # what specific version you have
```

On clusters or supercomputers which use environment modules to manage software packages, do this:

```
module list            # is a module for cmake already loaded?
module avail           # is a module for cmake available?
module load cmake3     # load cmake module with appropriate name
```

Most Linux distributions offer pre-compiled cmake packages through their package management system. If you do not have CMake or a new enough version, you can download the latest version at https://cmake.org/download/. Instructions on how to install it on various platforms can be found on this page.

3.2 Build LAMMPS with make

Building LAMMPS with traditional makefiles requires that you have a Makefile."machine" file appropriate for your system in the src/MAKE, src/MAKE/MACHINES, src/MAKE/OPTIONS, or src/MAKE/MINE directory (see below). It can include various options for customizing your LAMMPS build with a number of global compilation options and features.

Those makefiles are written for and tested with GNU make and may not be compatible with other make programs. In most cases, if the "make" program is not GNU make, then there will be a GNU make program available under the name "gmake". If GNU make or a compatible make is not available, you may have to first install it or switch to building with *CMake*. The makefiles of the traditional make based build process and the scripts they are calling expect a few additional tools to be available and functioning.

- a Bourne shell compatible "Unix" shell program (often this is bash)
- a few shell utilities: ls, mv, ln, rm, grep, sed, tr, cat, touch, diff, dirname
- python (optional, required for "make lib-XXX" in the src folder)

To include LAMMPS packages (i.e. optional commands and styles) you must enable them first, as discussed on the *Build package* doc page. If a packages requires (provided or external) libraries, you must configure and build those libraries **before** building LAMMPS itself and especially **before** enabling such a package with "make yes-<package>". Building *LAMMPS with CMake* can automate much of this for many types of machines, especially workstations, desktops, and laptops, so we suggest you try it first when building LAMMPS in those cases.

The commands below perform a default LAMMPS build, producing the LAMMPS executable lmp_serial and lmp_mpi in lammps/src:

```
cd lammps/src
make serial     # build a serial LAMMPS executable
make mpi        # build a parallel LAMMPS executable with MPI
make            # see a variety of make options
```

This initial compilation can take a long time, since LAMMPS is a large project with many features. If your machine has multiple CPU cores (most do these days), using a command like "make -jN mpi" (with N = the number of available CPU cores) can be much faster. If you plan to do development on LAMMPS or need to re-compile LAMMPS repeatedly, the installation of the ccache (= Compiler Cache) software may speed up compilation even more.

After the initial build, whenever you edit LAMMPS source files, or add or remove new files to the source directory (e.g. by installing or uninstalling packages), you must re-compile and relink the LAMMPS executable with the same "make" command. This makefiles dependencies should insure that only the subset of files that need to be are re-compiled.

Note: Before the actual compilation starts, LAMMPS will perform several steps to collect information from the configuration and setup that is then embedded into the executable. When you build LAMMPS for the first time, it will also compile a tool to quickly assemble a list of dependencies, that are required for the make program to correctly detect which parts need to be recompiled after changes were made to the sources.

The lammps/src/MAKE tree contains the Makefile.machine files included in the LAMMPS distribution. Typing "make machine" uses *Makefile.machine*. Thus the "make serial" or "make mpi" lines above use Makefile.serial and Makefile.mpi, respectively. Other makefiles are in these directories:

```
OPTIONS      # Makefiles which enable specific options
MACHINES     # Makefiles for specific machines
MINE         # customized Makefiles you create (you may need to create this folder)
```

Typing "make" lists all the available Makefile.machine files. A file with the same name can appear in multiple folders (not a good idea). The order the directories are searched is as follows: src/MAKE/MINE, src/MAKE, src/MAKE/OPTIONS, src/MAKE/MACHINES. This gives preference to a customized file you put in src/MAKE/MINE.

Makefiles you may wish to try include these (some require a package first be installed). Many of these include specific compiler flags for optimized performance. Please note, however, that some of these customized machine Makefile are contributed by users. Since both compilers, OS configurations, and LAMMPS itself keep changing, their settings may become outdated:

```
make mac             # build serial LAMMPS on a Mac
make mac_mpi         # build parallel LAMMPS on a Mac
make intel_cpu       # build with the USER-INTEL package optimized for CPUs
make knl             # build with the USER-INTEL package optimized for KNLs
make opt             # build with the OPT package optimized for CPUs
make omp             # build with the USER-OMP package optimized for OpenMP
make kokkos_omp      # build with the KOKKOS package for OpenMP
make kokkos_cuda_mpi # build with the KOKKOS package for GPUs
make kokkos_phi      # build with the KOKKOS package for KNLs
```

3.3 Link LAMMPS as a library to another code

LAMMPS can be used as a library by another application, including Python scripts. The files src/library.cpp and library.h define the C-style API for using LAMMPS as a library. See the *Howto library* doc page for a description of the interface and how to extend it for your needs.

The *Build basics* doc page explains how to build LAMMPS as either a shared or static library. This results in one of these 2 files:

```
liblammps.so      # shared library
liblammps.a       # static library
```

Note: Care should be taken to use the same MPI library for the calling code and the LAMMPS library. The library.h file includes mpi.h and uses definitions from it so those need to be available and consistent. When LAMMPS is compiled with the MPI STUBS library, then its mpi.h file needs to be included. While it is technically possible to use a full MPI library in the calling code and link to a serial LAMMPS library compiled with MPI STUBS, it is recommended to use the *same* MPI library for both, and then use MPI_Comm_split() in the calling code to pass a suitable communicator with a subset of MPI ranks to the function creating the LAMMPS instance.

Link with LAMMPS as a static library:

The calling application can link to LAMMPS as a static library with compilation and link commands as in the examples shown below. These are examples for a code written in C in the file *caller.c*. The benefit of linking to a static library is, that the resulting executable is independent of that library since all required executable code from the library is copied into the calling executable.

CMake build:

This assumes that LAMMPS has been configured with "-D BUILD_LIB=yes" and installed with "make install" and the PKG_CONFIG_PATH environment variable updated to include the *liblammps.pc* file installed into the configured destination folder, if needed. The commands to compile and link the coupled executable are then:

```
mpicc -c -O $(pkgconf liblammps --cflags) caller.c
mpicxx -o caller caller.o -$(pkgconf liblammps --libs)
```

Traditional make:

This assumes that LAMMPS has been compiled in the folder "${HOME}/lammps/src" with "make mode=lib mpi". The commands to compile and link the coupled executable are then:

```
mpicc -c -O -I${HOME}/lammps/src caller.c
mpicxx -o caller caller.o -L${HOME}/lammps/src -llammps
```

The *-I* argument is the path to the location of the *library.h* header file containing the interface to the LAMMPS C-style library interface. The *-L* argument is the path to where the *liblammps.a* file is located. The *-llammps* argument is shorthand for telling the compiler to link the file *liblammps.a*.

However, it is only as simple as shown above for the case of a plain LAMMPS library without any optional packages that depend on libraries (bundled or external). Otherwise, you need to include all flags, libraries, and paths for the coupled executable, that are also required to link the LAMMPS executable.

CMake build:

When using CMake, additional libraries with sources in the lib folder are built, but not included in liblammps.a and (currently) not installed with "make install" and not included in the *pkgconfig* configuration file. They can be found in the top level build folder, but you have to determine the necessary link flags manually. It is therefore recommended to either use the traditional make procedure to build and link with a static library or build and link with a shared library instead.

Traditional make:

After you have compiled a static LAMMPS library using the conventional build system for example with "make mode=lib serial". And you also have installed the POEMS package after building its bundled library in lib/poems. Then the commands to build and link the coupled executable change to:

```
gcc -c -O -I${HOME}/lammps/src/STUBS -I${HOME}/lammps/src -caller.c
g++ -o caller caller.o -L${HOME}/lammps/lib/poems \
  -L${HOME}/lammps/src/STUBS -L${HOME}/lammps/src -llammps -lpoems -lmpi_stubs
```

Note, that you need to link with "g++" instead of "gcc", since LAMMPS is C++ code. You can display the currently applied settings for building LAMMPS for the "serial" machine target by using the command:

```
make mode=print serial
```

Which should output something like:

```
# Compiler:
CXX=g++
# Linker:
LD=g++
# Compilation:
CXXFLAGS=-g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -I${HOME}/lammps/lib/poems -I${
↪{HOME}/lammps/src/STUBS
# Linking:
LDFLAGS=-g -O
# Libraries:
LDLIBS=-L${HOME}/lammps/lib/poems -L${HOME}/lammps/src/STUBS -lpoems -lmpi_stubs
```

From this you can gather the necessary paths and flags. With makefiles for other *machine* configurations you need to do the equivalent and replace "serial" with the corresponding *machine* name of the makefile.

Link with LAMMPS as a shared library:

When linking to LAMMPS built as a shared library, the situation becomes much simpler, as all dependent libraries and objects are included in the shared library, which is - technically speaking - effectively a regular LAMMPS executable that is missing the *main()* function. Thus those libraries need not to be specified when linking the calling executable. Only the *-I* flags are needed. So the example case from above of the serial version static LAMMPS library with the POEMS package installed becomes:

CMake build:

The commands with a shared LAMMPS library compiled with the CMake build process are the same as for the static library.

```
mpicc -c -O $(pkgconf liblammps --cflags) caller.c
mpicxx -o caller caller.o -$(pkgconf --libs)
```

Traditional make:

The commands with a shared LAMMPS library compiled with the traditional make build using "make mode=shlib serial" becomes:

```
gcc -c -O -I${HOME}/lammps/src/STUBS -I${HOME}/lammps/src -caller.c
g++ -o caller caller.o -L${HOME}/lammps/src -llammps
```

Locating liblammps.so at runtime:

However, now the *liblammps.so* file is required at runtime and needs to be in a folder, where the shared linker program of the operating system can find it. This would be either a folder like "/usr/local/lib64" or "${HOME}/.local/lib64" or a folder pointed to by the LD_LIBRARY_PATH environment variable. You can type

```
printenv LD_LIBRARY_PATH
```

to see what directories are in that list.

Or you can add the LAMMPS src directory (or the directory you performed a CMake style build in) to your LD_LIBRARY_PATH, so that the current version of the shared library is always available to programs that use it.

For the Bourne or Korn shells (/bin/sh, /bin/ksh, /bin/bash etc.), you would add something like this to your ~/.profile file:

```
LD_LIBRARY_PATH ${LD_LIBRARY_PATH-/usr/lib64}:${HOME}/lammps/src
export LD_LIBRARY_PATH
```

For the csh or tcsh shells, you would equivalently add something like this to your ~/.cshrc file:

```
setenv LD_LIBRARY_PATH ${LD_LIBRARY_PATH}:${HOME}/lammps/src
```

You can verify whether all required shared libraries are found with the *ldd* tool. Example:

```
$ LD_LIBRARY_PATH=/home/user/lammps/src ldd caller
     linux-vdso.so.1 (0x00007ffe729e0000)
     liblammps.so => /home/user/lammps/src/liblammps.so (0x00007fc91bb9e000)
     libstdc++.so.6 => /lib64/libstdc++.so.6 (0x00007fc91b984000)
     libm.so.6 => /lib64/libm.so.6 (0x00007fc91b83e000)
     libgcc_s.so.1 => /lib64/libgcc_s.so.1 (0x00007fc91b824000)
     libc.so.6 => /lib64/libc.so.6 (0x00007fc91b65b000)
     /lib64/ld-linux-x86-64.so.2 (0x00007fc91c094000)
```

If a required library is missing, you would get a 'not found' entry:

```
$  ldd caller
     linux-vdso.so.1 (0x00007ffd672fe000)
     liblammps.so => not found
     libstdc++.so.6 => /usr/lib64/libstdc++.so.6 (0x00007fb7c7e86000)
     libm.so.6 => /usr/lib64/libm.so.6 (0x00007fb7c7d40000)
     libgcc_s.so.1 => /usr/lib64/libgcc_s.so.1 (0x00007fb7c7d26000)
     libc.so.6 => /usr/lib64/libc.so.6 (0x00007fb7c7b5d000)
     /lib64/ld-linux-x86-64.so.2 (0x00007fb7c80a2000)
```

Calling the LAMMPS library:

Either flavor of library (static or shared) allows one or more LAMMPS objects to be instantiated from the calling program. When used from a C++ program, most of the symbols and functions in LAMMPS are wrapped in a LAMMPS_NS namespace; you can safely use any of its classes and methods from within the calling code, as needed, and you will not incur conflicts with functions and variables in your code that share the name. This, however, does not extend to all additional libraries bundled with LAMMPS in the lib folder and some of the low-level code of some packages.

To be compatible with C, Fortran, Python programs, the library has a simple C-style interface, provided in src/library.cpp and src/library.h.

See the *Python library* doc page for a description of the Python interface to LAMMPS, which wraps the C-style interface from a shared library through the ctypes python module.

See the sample codes in examples/COUPLE/simple for examples of C++ and C and Fortran codes that invoke LAMMPS through its library interface. Other examples in the COUPLE directory use coupling ideas discussed on the *Howto couple* doc page.

3.4 Basic build options

The following topics are covered on this page, for building both with CMake and make:

- *Serial vs parallel build*
- *Choice of compiler and compile/link options*
- *Build LAMMPS as an executable or a library*
- *Build the LAMMPS documentation*
- *Install LAMMPS after a build*

3.4.1 Serial vs parallel build

LAMMPS is written to use the ubiquitous MPI (Message Passing Interface) library API for distributed memory parallel computation. You need to have such a library installed for building and running LAMMPS in parallel using a domain decomposition parallelization. It is compatible with the MPI standard version 2.x and later. LAMMPS can also be built into a "serial" executable for use with a single processor using the bundled MPI STUBS library.

Independent of the distributed memory MPI parallelization, parts of LAMMPS are also written with support for shared memory parallelization using the OpenMP threading standard. A more detailed discussion of that is below.

CMake build:

```
-D BUILD_MPI=value          # yes or no, default is yes if CMake finds MPI, else no
-D BUILD_OMP=value          # yes or no, default is yes if a compatible compiler is␣
↪detected
-D LAMMPS_MACHINE=name      # name = mpi, serial, mybox, titan, laptop, etc
                            # no default value
```

The executable created by CMake (after running make) is named *lmp* unless the LAMMPS_MACHINE option is set. When setting *LAMMPS_MACHINE=name* the executable will be named *lmp_name*. Using *BUILD_MPI=no* will enforce building a serial executable using the MPI STUBS library.

Traditional make:

The build with traditional makefiles has to be done inside the source folder *src*.

```
make mpi                # parallel build, produces lmp_mpi using Makefile.mpi
make serial             # serial build, produces lmp_serial using Makefile/serial
make mybox              # uses Makefile.mybox to produce lmp_mybox
```

Any "make machine" command will look up the make settings from a file Makefile.machine, create a folder Obj_machine with all objects and generated files and an executable called *lmp_machine*. The standard parallel build with *make mpi* assumes a standard MPI installation with MPI compiler wrappers where all necessary compiler and linker flags to get access and link with the suitable MPI headers and libraries are set by the wrapper programs. For other cases or the serial build, you have to adjust the make file variables MPI_INC, MPI_PATH, MPI_LIB as well as CC and LINK. To enable OpenMP threading usually a compiler specific flag needs to be added to the compile and link commands. For the GNU compilers, this is *-fopenmp*, which can be added to the CC and LINK makefile variables.

For the serial build the following make variables are set (see src/MAKE/Makefile.serial):

```
CC =            g++
LINK =          g++
MPI_INC =       -I../STUBS
MPI_PATH =      -L../STUBS
MPI_LIB =       -lmpi_stubs
```

You also need to build the STUBS library for your platform before making LAMMPS itself. A "make serial" build does this for you automatically, otherwise, type "make mpi-stubs" from the src directory, or "make" from the src/STUBS dir. If the build fails, you will need to edit the STUBS/Makefile for your platform. The stubs library does not provide MPI/IO functions required by some LAMMPS packages, e.g. MPIIO or USER-LB, and thus is not compatible with those packages.

Note: The file STUBS/mpi.c provides a CPU timer function called MPI_Wtime() that calls gettimeofday() . If your operating system does not support gettimeofday() , you will need to insert code to call another timer. Note that the ANSI-standard function clock() rolls over after an hour or so, and is therefore insufficient for timing long LAMMPS simulations.

MPI and OpenMP support info:

If you are installing MPI yourself to build a parallel LAMMPS executable, we recommend either MPICH or OpenMPI which are regularly used and tested with LAMMPS by the LAMMPS developers. MPICH can be downloaded from the MPICH home page and OpenMPI can be downloaded correspondingly from the OpenMPI home page. Other MPI packages should also work. No specific vendor provided and standard compliant MPI library is currently known to be incompatible with LAMMPS. If you are running on a large parallel machine, your system admins or the vendor should have already installed a version of MPI, which is likely to be faster than a self-installed MPICH or OpenMPI, so you should study the provided documentation to find out how to build and link with it.

The majority of OpenMP (threading) support in LAMMPS is provided by the USER-OMP package; see the *Speed omp*

doc page for details. The USER-INTEL package also includes OpenMP threading (it is compatible with USER-OMP) and adds vectorization support when compiled with compatible compilers, in particular the Intel compilers on top of OpenMP. Also, the KOKKOS package can be compiled to include OpenMP threading.

In addition, there are a few commands in LAMMPS that have native OpenMP support included as well. These are commands in the MPIIO, SNAP, USER-DIFFRACTION, and USER-DPD packages. In addition some packages support OpenMP threading indirectly through the libraries they interface to: e.g. LATTE and USER-COLVARS. See the *Packages details* doc page for more info on these packages and the doc pages for their respective commands for OpenMP threading info.

For CMake, if you use BUILD_OMP=yes, you can use these packages and turn on their native OpenMP support and turn on their native OpenMP support at run time, by setting the OMP_NUM_THREADS environment variable before you launch LAMMPS.

For building via conventional make, the CCFLAGS and LINKFLAGS variables in Makefile.machine need to include the compiler flag that enables OpenMP. For GNU compilers it is -fopenmp. For (recent) Intel compilers it is -qopenmp. If you are using a different compiler, please refer to its documentation.

OpenMP Compiler compatibility info:

Some compilers do not fully support the 'default(none)' directive and others (e.g. GCC version 9 and beyond) may implement OpenMP 4.0 semantics, which are incompatible with the OpenMP 3.1 directives used in LAMMPS (for maximal compatibility with compiler versions in use). In those case, all 'default(none)' directives (which aid in detecting incorrect and unwanted sharing) can be replaced with 'default(shared)' while dropping all 'shared()' directives. The script 'src/USER-OMP/hack_openmp_for_pgi_gcc9.sh' can be used to automate this conversion.

3.4.2 Choice of compiler and compile/link options

The choice of compiler and compiler flags can be important for performance. Vendor provided compilers for a specific hardware can produce faster code than open-source compilers like the GNU compilers. On x86 hardware most popular compilers are quite similar in performance of C/C++ code at high optimization levels. When using the USER-INTEL package, there is a distinct advantage in using the Intel C++ compiler due to much improved vectorization through SSE and AVX instructions on compatible hardware as the source code includes changes and compiler directives to enable high degrees of vectorization.

On parallel clusters or supercomputers which use "environment modules" for their compile/link environments, you can often access different compilers by simply loading the appropriate module before building LAMMPS.

CMake build:

By default CMake will use a compiler it finds and it will add optimization flags appropriate to that compiler and any *accelerator packages* you have included in the build.

You can tell CMake to look for a specific compiler with these variable settings. Likewise you can specify the FLAGS variables if you want to experiment with alternate optimization flags. You should specify all 3 compilers, so that the small number of LAMMPS source files written in C or Fortran are built with a compiler consistent with the one used for all the C++ files:

```
-D CMAKE_CXX_COMPILER=name            # name of C++ compiler
-D CMAKE_C_COMPILER=name              # name of C compiler
-D CMAKE_Fortran_COMPILER=name        # name of Fortran compiler

-D CMAKE_CXX_FLAGS=string             # flags to use with C++ compiler
-D CMAKE_C_FLAGS=string               # flags to use with C compiler
-D CMAKE_Fortran_FLAGS=string         # flags to use with Fortran compiler
```

A few example command lines are:

```
# Building with GNU Compilers:
cmake ../cmake -DCMAKE_C_COMPILER=gcc -DCMAKE_CXX_COMPILER=g++ -DCMAKE_Fortran_
↪COMPILER=gfortran
# Building with Intel Compilers:
cmake ../cmake -DCMAKE_C_COMPILER=icc -DCMAKE_CXX_COMPILER=icpc -DCMAKE_Fortran_
↪COMPILER=ifort
# Building with LLVM/Clang Compilers:
cmake ../cmake -DCMAKE_C_COMPILER=clang -DCMAKE_CXX_COMPILER=clang++ -DCMAKE_Fortran_
↪COMPILER=flang
```

For compiling with the Clang/LLVM compilers a special CMake preset is included that can be loaded with *-C ../cmake/presets/clang.cmake*.

Note: When the cmake command completes, it prints a summary to the screen which compilers it is using and what flags and settings will be used for the compilation. Note that if the top-level compiler is mpicxx, it is simply a wrapper on a real compiler. The underlying compiler info is what CMake will try to determine and report. You should check to confirm you are using the compiler and optimization flags you want.

Makefile.machine settings for traditional make:

The "compiler/linker settings" section of a Makefile.machine lists compiler and linker settings for your C++ compiler, including optimization flags. For a parallel build it is recommended to use mpicxx or mpiCC, since these compiler wrappers will include a variety of settings appropriate for your MPI installation and thus avoiding the guesswork of finding the right flags.

Parallel build (see src/MAKE/Makefile.mpi):

```
CC =            mpicxx
CCFLAGS =       -g -O3
LINK =          mpicxx
LINKFLAGS =     -g -O
```

Serial build (see src/MAKE/Makefile.serial):

```
CC =            g++
CCFLAGS =       -g -O3
LINK =          g++
LINKFLAGS =     -g -O
```

Note: If you build LAMMPS with any *accelerator packages* included, there may be specific optimization flags that are either required or recommended to enable required features and to achieve optimal performance. You need to include these in the CCFLAGS and LINKFLAGS settings above. For details, see the individual package doc pages listed on the *Speed packages* doc page. Or examine these files in the src/MAKE/OPTIONS directory. They correspond to each of the 5 accelerator packages and their hardware variants:

```
Makefile.opt                    # OPT package
Makefile.omp                    # USER-OMP package
Makefile.intel_cpu              # USER-INTEL package for CPUs
Makefile.intel_coprocessor      # USER-INTEL package for KNLs
Makefile.gpu                    # GPU package
Makefile.kokkos_cuda_mpi        # KOKKOS package for GPUs
Makefile.kokkos_omp             # KOKKOS package for CPUs (OpenMP)
Makefile.kokkos_phi             # KOKKOS package for KNLs (OpenMP)
```

3.4.3 Build LAMMPS as an executable or a library

LAMMPS can be built as either an executable or as a static or shared library. The LAMMPS library can be called from another application or a scripting language. See the *Howto couple* doc page for more info on coupling LAMMPS to other codes. See the *Python* doc page for more info on wrapping and running LAMMPS from Python via its library interface.

CMake build:

For CMake builds, you can select through setting CMake variables which files the compilation produces during the configuration step. If none are set, defaults are applied.

```
-D BUILD_EXE=value            # yes (default) or no
-D BUILD_LIB=value            # yes or no (default)
-D BUILD_SHARED_LIBS=value    # yes or no (default)
-D LAMMPS_LIB_SUFFIX=name     # name = mpi, serial, mybox, titan, laptop, etc
                              # no default value
```

Setting BUILD_EXE=no will not produce an executable. Setting BUILD_LIB=yes will produce a static library named *liblammps.a*. Setting both BUILD_LIB=yes and BUILD_SHARED_LIBS=yes will produce a shared library named *liblammps.so* instead. If LAMMPS_LIB_SUFFIX is set to *name* in addition, the name of the generated libraries will be changed to either *liblammps_name.a* or *liblammps_name.so*, respectively.

Traditional make:

With the traditional makefile based build process, the choice of the generated executable or library depends on the "mode" setting. Several options are available and "mode=exe" is the default.

```
make machine                # build LAMMPS executable lmp_machine
mkae mode=exe machine       # same as "make machine"
make mode=lib machine       # build LAMMPS static lib liblammps_machine.a
make mode=shlib machine     # build LAMMPS shared lib liblammps_machine.so
make mode=shexe machine     # same as "mode=exe" but uses objects from "mode=shlib"
```

The two "exe" builds will generate and executable *lmp_machine*, while the two library builds will create a file *liblammps_machine.a* or *liblammps_machine.so*. They will also create generic soft links, named *liblammps.a* and *liblammps.so*, which point to the specific *liblammps_machine.a/so* files.

CMake and make info:

Note that for a shared library to be usable by a calling program, all the auxiliary libraries it depends on must also exist as shared libraries. This will be the case for libraries included with LAMMPS, such as the dummy MPI library in src/STUBS or any package libraries in the lib/packages directory, since they are always built in a shared library compatible way using the -fPIC switch. However, if a library like MPI or FFTW does not exist as a shared library, the shared library build may generate an error. This means you will need to install a shared library version of the auxiliary library. The build instructions for the library should tell you how to do this.

As an example, here is how to build and install the MPICH library, a popular open-source version of MPI, as a shared library in the default /usr/local/lib location:

```
./configure --enable-shared
make
make install
```

You may need to use "sudo make install" in place of the last line if you do not have write privileges for /usr/local/lib. The end result should be the file /usr/local/lib/libmpich.so. On many Linux installations the folder "${HOME}/.local"

is an alternative to using /usr/local and does not require superuser or sudo access. In that case the configuration step becomes:

```
./configure --enable-shared --prefix=${HOME}/.local
```

Avoiding using "sudo" for custom software installation (i.e. from source and not through a package manager tool provided by the OS) is generally recommended to ensure the integrity of the system software installation.

3.4.4 Build the LAMMPS documentation

The LAMMPS manual is written in reStructuredText format which can be translated to different output format using the Sphinx document generator tool. Currently the translation to HTML and PDF (via LaTeX) are supported. For that to work a Python 3 interpreter and internet access is required. For the documentation build a python based virtual environment is set up in the folder doc/docenv and various python packages are installed into that virtual environment via the pip tool. The actual translation is then done via make commands.

Documentation make option:

The following make commands can be issued in the doc folder of the LAMMPS source distribution.

```
make html          # create HTML doc pages in html directory
make pdf           # create Developer.pdf and Manual.pdf in this directory
make fetch         # fetch HTML and PDF files from LAMMPS web site
make clean         # remove all intermediate files
make clean-all     # reset the entire doc build environment
make anchor_check  # scan for duplicate anchor labels
make style_check   # check for complete and consistent style lists
make package_check # check for complete and consistent package lists
make spelling      # spell-check the manual
```

Thus "make html" will create a "doc/html" directory with the HTML format manual pages so that you can browse them with a web browser locally on your system.

Note: You can also download a tarball of the documentation for the current LAMMPS version (HTML and PDF files), from the website download page.

CMake build option:

It is also possible to create the HTML version of the manual within the *CMake build directory*. The reason for this option is to include the installation of the HTML manual pages into the "install" step when installing LAMMPS after the CMake build via "make install".

```
-D BUILD_DOC=value        # yes or no (default)
```

3.4.5 Build LAMMPS tools

Some tools described in *Auxiliary tools* can be built directly using CMake or Make.

CMake build3:

```
-D BUILD_TOOLS=value       # yes or no (default)
```

The generated binaries will also become part of the LAMMPS installation (see below).

Traditional make:

```
cd lammps/tools
make all              # build all binaries of tools
make binary2txt       # build only binary2txt tool
make chain            # build only chain tool
make micelle2d        # build only micelle2d tool
make thermo_extract   # build only thermo_extract tool
```

3.4.6 Install LAMMPS after a build

After building LAMMPS, you may wish to copy the LAMMPS executable of library, along with other LAMMPS files (library header, doc files) to a globally visible place on your system, for others to access. Note that you may need super-user privileges (e.g. sudo) if the directory you want to copy files to is protected.

CMake build:

```
cmake -D CMAKE_INSTALL_PREFIX=path [options ...] ../cmake
make                        # perform make after CMake command
make install                # perform the installation into prefix
```

Traditional make:

There is no "install" option in the src/Makefile for LAMMPS. If you wish to do this you will need to first build LAMMPS, then manually copy the desired LAMMPS files to the appropriate system directories.

3.5 Optional build settings

LAMMPS can be built with several optional settings. Each sub-section explain how to do this for building both with CMake and make.

- *C++11 standard compliance* when building all of LAMMPS
- *FFT library* for use with the *kspace_style pppm* command
- *Size of LAMMPS data types*
- *Read or write compressed files*
- *Output of JPG and PNG files* via the *dump image* command
- *Output of movie files* via the *dump_movie* command
- *Memory allocation alignment*
- *Workaround for long long integers*

- *Error handling exceptions* when using LAMMPS as a library

3.5.1 C++11 standard compliance

The LAMMPS developers plan to transition to make the C++11 standard the minimum requirement for compiling LAMMPS. Currently this only applies to some packages like KOKKOS while the rest aims to be compatible with the C++98 standard. Most currently used compilers are compatible with C++11; some need to set extra flags to enable C++11 compliance. Example for GNU c++:

```
CCFLAGS = -g -O3 -std=c++11
```

3.5.2 FFT library

When the KSPACE package is included in a LAMMPS build, the *kspace_style pppm* command performs 3d FFTs which require use of an FFT library to compute 1d FFTs. The KISS FFT library is included with LAMMPS but other libraries can be faster. LAMMPS can use them if they are available on your system.

CMake variables:

```
-D FFT=value              # FFTW3 or MKL or KISS, default is FFTW3 if found, else KISS
-D FFT_SINGLE=value       # yes or no (default), no = double precision
-D FFT_PACK=value         # array (default) or pointer or memcpy
```

Note: The values for the FFT variable must be in upper-case. This is an exception to the rule that all CMake variables can be specified with lower-case values.

Usually these settings are all that is needed. If FFTW3 is selected, then CMake will try to detect, if threaded FFTW libraries are available and enable them by default. This setting is independent of whether OpenMP threads are enabled and a packages like KOKKOS or USER-OMP is used. If CMake cannot detect the FFT library, you can set these variables to assist:

```
-D FFTW3_INCLUDE_DIRS=path  # path to FFTW3 include files
-D FFTW3_LIBRARIES=path     # path to FFTW3 libraries
-D FFT_FFTW_THREADS=on      # enable using threaded FFTW3 libraries
-D MKL_INCLUDE_DIRS=path    # ditto for Intel MKL library
-D FFT_MKL_THREADS=on       # enable using threaded FFTs with MKL libraries
-D MKL_LIBRARIES=path
```

Makefile.machine settings:

```
FFT_INC = -DFFT_FFTW3         # -DFFT_FFTW3, -DFFT_FFTW (same as -DFFT_FFTW3), -DFFT_
↪MKL, or -DFFT_KISS
                              # default is KISS if not specified
FFT_INC = -DFFT_SINGLE        # do not specify for double precision
FFT_INC = -DFFT_FFTW_THREADS  # enable using threaded FFTW3 libraries
FFT_INC = -DFFT_MKL_THREADS   # enable using threaded FFTs with MKL libraries
FFT_INC = -DFFT_PACK_ARRAY    # or -DFFT_PACK_POINTER or -DFFT_PACK_MEMCPY
```

default is FFT_PACK_ARRAY if not specified

```
FFT_INC =       -I/usr/local/include
FFT_PATH =      -L/usr/local/lib
FFT_LIB =       -lfftw3             # FFTW3 double precision
FFT_LIB =       -lfftw3 -lfftw3_omp # FFTW3 double precision with threads (needs -
↪DFFT_FFTW_THREADS)
FFT_LIB =       -lfftw3 -lfftw3f    # FFTW3 single precision
FFT_LIB =       -lmkl_intel_lp64 -lmkl_sequential -lmkl_core   # MKL with Intel␣
↪compiler, serial interface
FFT_LIB =       -lmkl_gf_lp64 -lmkl_sequential -lmkl_core      # MKL with GNU compier,
↪ serial interface
FFT_LIB =       -lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core # MKL with Intel␣
↪compiler, threaded interface
FFT_LIB =       -lmkl_gf_lp64 -lmkl_gnu_thread -lmkl_core      # MKL with GNU␣
↪compiler, threaded interface
FFT_LIB =       -lmkl_rt            # MKL with automatic runtime selection of␣
↪interface libs
```

As with CMake, you do not need to set paths in FFT_INC or FFT_PATH, if the compiler can find the FFT header and library files in its default search path. You must specify FFT_LIB with the appropriate FFT libraries to include in the link.

CMake and make info:

The KISS FFT library is included in the LAMMPS distribution. It is portable across all platforms. Depending on the size of the FFTs and the number of processors used, the other libraries listed here can be faster.

However, note that long-range Coulombics are only a portion of the per-timestep CPU cost, FFTs are only a portion of long-range Coulombics, and 1d FFTs are only a portion of the FFT cost (parallel communication can be costly). A breakdown of these timings is printed to the screen at the end of a run when using the *kspace_style pppm* command. The *Run output* doc page gives more details. A more detailed (and time consuming) report of the FFT performance is generated with the *kspace_modify fftbench yes* command.

FFTW is a fast, portable FFT library that should also work on any platform and can be faster than the KISS FFT library. You can download it from www.fftw.org. LAMMPS requires version 3.X; the legacy version 2.1.X is no longer supported.

Building FFTW for your box should be as simple as ./configure; make; make install. The install command typically requires root privileges (e.g. invoke it via sudo), unless you specify a local directory with the "–prefix" option of configure. Type "./configure –help" to see various options.

The Intel MKL math library is part of the Intel compiler suite. It can be used with the Intel or GNU compiler (see FFT_LIB setting above).

Performing 3d FFTs in parallel can be time consuming due to data access and required communication. This cost can be reduced by performing single-precision FFTs instead of double precision. Single precision means the real and imaginary parts of a complex datum are 4-byte floats. Double precision means they are 8-byte doubles. Note that Fourier transform and related PPPM operations are somewhat less sensitive to floating point truncation errors and thus the resulting error is less than the difference in precision. Using the -DFFT_SINGLE setting trades off a little accuracy for reduced memory use and parallel communication costs for transposing 3d FFT data.

When using -DFFT_SINGLE with FFTW3 you may need to build the FFTW library a second time with support for single-precision.

For FFTW3, do the following, which should produce the additional library libfftw3f.a or libfftw3f.so.

```
make clean
./configure --enable-single; make; make install
```

Performing 3d FFTs requires communication to transpose the 3d FFT grid. The data packing/unpacking for this can be done in one of 3 modes (ARRAY, POINTER, MEMCPY) as set by the FFT_PACK syntax above. Depending on

the machine, the size of the FFT grid, the number of processors used, one option may be slightly faster. The default is ARRAY mode.

3.5.3 Size of LAMMPS data types

LAMMPS has a few integer data types which can be defined as 4-byte or 8-byte integers. The default setting of "smallbig" is almost always adequate.

CMake variable:

```
-D LAMMPS_SIZES=value   # smallbig (default) or bigbig or smallsmall
```

Makefile.machine setting:

```
LMP_INC = -DLAMMPS_SMALLBIG    # or -DLAMMPS_BIGBIG or -DLAMMPS_SMALLSMALL
```

default is LAMMPS_SMALLBIG if not specified **CMake and make info**:

The default "smallbig" setting allows for simulations with:

- total atom count = 2^63 atoms (about 9e18)
- total timesteps = 2^63 (about 9e18)
- atom IDs = 2^31 (about 2 billion)
- image flags = roll over at 512

The "bigbig" setting increases the latter two limits. It allows for:

- total atom count = 2^63 atoms (about 9e18)
- total timesteps = 2^63 (about 9e18)
- atom IDs = 2^63 (about 9e18)
- image flags = roll over at about 1 million (2^20)

The "smallsmall" setting is only needed if your machine does not support 8-byte integers. It allows for:

- total atom count = 2^31 atoms (about 2 billion)
- total timesteps = 2^31 (about 2 billion)
- atom IDs = 2^31 (about 2 billion)
- image flags = roll over at 512 (2^9)

Atom IDs are not required for atomic systems which do not store bond topology information, though IDs are enabled by default. The *atom_modify id no* command will turn them off. Atom IDs are required for molecular systems with bond topology (bonds, angles, dihedrals, etc). Thus if you model a molecular system with more than 2 billion atoms, you need the "bigbig" setting.

Image flags store 3 values per atom which count the number of times an atom has moved through the periodic box in each dimension. See the *dump* doc page for a discussion. If an atom moves through the periodic box more than this limit, the value will "roll over", e.g. from 511 to -512, which can cause diagnostics like the mean-squared displacement, as calculated by the *compute msd* command, to be faulty.

Note that the USER-ATC package and the USER-INTEL package are currently not compatible with the "bigbig" setting. Also, there are limitations when using the library interface. Some functions with known issues have been replaced by dummy calls printing a corresponding error rather than crashing randomly or corrupting data.

Also note that the GPU package requires its lib/gpu library to be compiled with the same size setting, or the link will fail. A CMake build does this automatically. When building with make, the setting in whichever lib/gpu/Makefile is used must be the same as above.

3.5.4 Output of JPG, PNG, and movie files

The *dump image* command has options to output JPEG or PNG image files. Likewise the *dump movie* command outputs movie files in MPEG format. Using these options requires the following settings:

CMake variables:

```
-D WITH_JPEG=value       # yes or no
                         # default = yes if CMake finds JPEG files, else no
-D WITH_PNG=value        # yes or no
                         # default = yes if CMake finds PNG and ZLIB files, else no
-D WITH_FFMPEG=value     # yes or no
                         # default = yes if CMake can find ffmpeg, else no
```

Usually these settings are all that is needed. If CMake cannot find the graphics header, library, executable files, you can set these variables:

```
-D JPEG_INCLUDE_DIR=path     # path to jpeglib.h header file
-D JPEG_LIBRARIES=path       # path to libjpeg.a (.so) file
-D PNG_INCLUDE_DIR=path      # path to png.h header file
-D PNG_LIBRARIES=path        # path to libpng.a (.so) file
-D ZLIB_INCLUDE_DIR=path     # path to zlib.h header file
-D ZLIB_LIBRARIES=path       # path to libz.a (.so) file
-D FFMPEG_EXECUTABLE=path    # path to ffmpeg executable
```

Makefile.machine settings:

```
LMP_INC = -DLAMMPS_JPEG
LMP_INC = -DLAMMPS_PNG
LMP_INC = -DLAMMPS_FFMPEG

JPG_INC = -I/usr/local/include   # path to jpeglib.h, png.h, zlib.h header files if␣
↪make cannot find them
JPG_PATH = -L/usr/lib            # paths to libjpeg.a, libpng.a, libz.a (.so) files␣
↪if make cannot find them
JPG_LIB = -ljpeg -lpng -lz       # library names
```

As with CMake, you do not need to set JPG_INC or JPG_PATH, if make can find the graphics header and library files. You must specify JPG_LIB with a list of graphics libraries to include in the link. You must insure ffmpeg is in a directory where LAMMPS can find it at runtime, that is a directory in your PATH environment variable.

CMake and make info:

Using ffmpeg to output movie files requires that your machine supports the "popen" function in the standard runtime library.

Note: On some clusters with high-speed networks, using the fork() library call (required by popen()) can interfere with the fast communication library and lead to simulations using ffmpeg to hang or crash.

3.5.5 Read or write compressed files

If this option is enabled, large files can be read or written with gzip compression by several LAMMPS commands, including *read_data*, *rerun*, and *dump*.

CMake variables:

```
-D WITH_GZIP=value        # yes or no
                          # default is yes if CMake can find gzip, else no
-D GZIP_EXECUTABLE=path   # path to gzip executable if CMake cannot find it
```

Makefile.machine setting:

```
LMP_INC = -DLAMMPS_GZIP
```

CMake and make info:

This option requires that your machine supports the "popen()" function in the standard runtime library and that a gzip executable can be found by LAMMPS during a run.

Note: On some clusters with high-speed networks, using the fork() library call (required by popen()) can interfere with the fast communication library and lead to simulations using compressed output or input to hang or crash. For selected operations, compressed file I/O is also available using a compression library instead, which is what the *COMPRESS package* enables.

3.5.6 Memory allocation alignment

This setting enables the use of the posix_memalign() call instead of malloc() when LAMMPS allocates large chunks or memory. This can make vector instructions on CPUs more efficient, if dynamically allocated memory is aligned on larger-than-default byte boundaries. On most current systems, the malloc() implementation returns pointers that are aligned to 16-byte boundaries. Using SSE vector instructions efficiently, however, requires memory blocks being aligned on 64-byte boundaries.

CMake variable:

```
-D LAMMPS_MEMALIGN=value            # 0, 8, 16, 32, 64 (default)
```

Use a LAMMPS_MEMALIGN value of 0 to disable using posix_memalign() and revert to using the malloc() C-library function instead. When compiling LAMMPS for Windows systems, malloc() will always be used and this setting ignored.

Makefile.machine setting:

```
LMP_INC = -DLAMMPS_MEMALIGN=value   # 8, 16, 32, 64
```

Do not set -DLAMMPS_MEMALIGN, if you want to have memory allocated with the malloc() function call instead. -DLAMMPS_MEMALIGN **cannot** be used on Windows, as it does use different function calls for allocating aligned memory, that are not compatible with how LAMMPS manages its dynamical memory.

3.5.7 Workaround for long long integers

If your system or MPI version does not recognize "long long" data types, the following setting will be needed. It converts "long long" to a "long" data type, which should be the desired 8-byte integer on those systems:

CMake variable:

```
-D LAMMPS_LONGLONG_TO_LONG=value      # yes or no (default)
```

Makefile.machine setting:

```
LMP_INC = -DLAMMPS_LONGLONG_TO_LONG
```

3.5.8 Exception handling when using LAMMPS as a library

This setting is useful when external codes drive LAMMPS as a library. With this option enabled, LAMMPS errors do not kill the calling code. Instead, the call stack is unwound and control returns to the caller, e.g. to Python. Of course the calling code has to be set up to *catch* exceptions from within LAMMPS.

CMake variable:

```
-D LAMMPS_EXCEPTIONS=value        # yes or no (default)
```

Makefile.machine setting:

```
LMP_INC = -DLAMMPS_EXCEPTIONS
```

3.6 Include packages in build

In LAMMPS, a package is a group of files that enable a specific set of features. For example, force fields for molecular systems or rigid-body constraints are in packages. In the src directory, each package is a sub-directory with the package name in capital letters.

An overview of packages is given on the *Packages* doc page. Brief overviews of each package are on the *Packages details* doc page.

When building LAMMPS, you can choose to include or exclude each package. In general there is no need to include a package if you never plan to use its features.

If you get a run-time error that a LAMMPS command or style is "unknown", it is often because the command is contained in a package, and your build did not include that package. If the command or style *is* available in a package included in the LAMMPS distribution, the error message will indicate which package would be needed. Running LAMMPS with the *-h command-line switch* will print *all* optional commands and packages that were enabled when building that executable.

For the majority of packages, if you follow the single step below to include it, you can then build LAMMPS exactly the same as you would without any packages installed. A few packages may require additional steps, as explained on the *Build extras* doc page.

These links take you to the extra instructions for those select packages:

COMPRESS	*GPU*	*KIM*	*KOKKOS*	*LATTE*	*MESSAGE*
MSCG	*OPT*	*POEMS*	*PYTHON*	*VORONOI*	*USER-ADIOS*
USER-ATC	*USER-AWPMD*	*USER-COLVARS*	*USER-H5MD*	*USER-INTEL*	*USER-MOLFILE*
USER-NETCDF	*USER-PLUMED*	*USER-OMP*	*USER-QMMM*	*USER-QUIP*	*USER-SCAFACOS*
USER-SMD	*USER-VTK*				

The mechanism for including packages is simple but different for CMake versus make.

CMake build:

```
-D PKG_NAME=value           # yes or no (default)
```

Examples:

```
-D PKG_MANYBODY=yes
-D PKG_USER-INTEL=yes
```

All standard and user packages are included the same way. Note that USER packages have a hyphen between USER and the rest of the package name, not an underscore.

See the shortcut section below for how to install many packages at once with CMake.

Note: If you toggle back and forth between building with CMake vs make, no packages in the src directory can be installed when you invoke cmake. CMake will give an error if that is not the case, indicating how you can un-install all packages in the src dir.

Traditional make:

```
cd lammps/src
make ps                     # check which packages are currently installed
make yes-name               # install a package with name
make no-name                # un-install a package with name
make mpi                    # build LAMMPS with whatever packages are now installed
```

Examples:

```
make no-rigid
make yes-user-intel
```

All standard and user packages are included the same way.

See the shortcut section below for how to install many packages at once with make.

Note: You must always re-build LAMMPS (via make) after installing or un-installing a package, for the action to take effect.

Note: You cannot install or un-install packages and build LAMMPS in a single make command with multiple targets, e.g. make yes-colloid mpi. This is because the make procedure creates a list of source files that will be out-of-date for the build if the package configuration changes within the same command. You can include or exclude multiple packages in a single make command, e.g. make yes-colloid no-manybody.

CMake and make info:

Any package can be included or excluded in a LAMMPS build, independent of all other packages. However, some packages include files derived from files in other packages. LAMMPS checks for this and does the right thing. Individual files are only included if their dependencies are already included. Likewise, if a package is excluded, other files dependent on that package are also excluded.

When you download a LAMMPS tarball or download LAMMPS source files from the git repository, no packages are pre-installed in the src directory.

Note: Prior to Aug 2018, if you downloaded a tarball, 3 packages (KSPACE, MANYBODY, MOLECULE) were pre-installed in the src directory. That is no longer the case, so that CMake will build as-is without the need to un-install those packages.

CMake shortcuts for installing many packages:

Instead of specifying all the CMake options via the command-line, CMake allows initializing its settings cache using script files. These are regular CMake files which can manipulate and set CMake variables (which represent selected options), and can also contain control flow constructs for more complex operations.

LAMMPS includes several of these files to define configuration "presets", similar to the options that exist for the Make based system. Using these files you can enable/disable portions of the available packages in LAMMPS. If you need a custom preset you can take one of them as a starting point and customize it to your needs.

```
cmake -C ../cmake/presets/all_on.cmake  [OPTIONS] ../cmake  # enable all packages
cmake -C ../cmake/presets/all_off.cmake [OPTIONS] ../cmake  # disable all packages
cmake -C ../cmake/presets/minimal.cmake [OPTIONS] ../cmake  # enable just a few core␣
↪packages
cmake -C ../cmake/presets/most.cmake    [OPTIONS] ../cmake  # enable most common␣
↪packages
cmake -C ../cmake/presets/nolib.cmake   [OPTIONS] ../cmake  # disable packages that␣
↪do require extra libraries or tools
cmake -C ../cmake/presets/clang.cmake   [OPTIONS] ../cmake  # change settings to use␣
↪the Clang compilers by default
cmake -C ../cmake/presets/mingw.cmake   [OPTIONS] ../cmake  # enable all packages␣
↪compatible with MinGW compilers
```

Note: Running cmake this way manipulates the CMake settings cache in your current build directory. You can combine multiple presets and options in a single cmake run, or change settings incrementally by running cmake with new flags.

Example:

```
# build LAMMPS with most commonly used packages, but then remove
# those requiring additional library or tools, but still enable
# GPU package and configure it for using CUDA. You can run.
mkdir build
cd build
cmake -C ../cmake/presets/most.cmake -C ../cmake/presets/nolib.cmake -D PKG_GPU=on -D␣
↪GPU_API=cuda ../cmake

# to add another package, say BODY to the previous configuration you can run:
cmake -D PKG_BODY=on .
```

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```
# to reset the package selection from above to the default of no packages
# but leaving all other settings untouched. You can run:
cmake -C ../cmake/presets/no_all.cmake .
```

Make shortcuts for installing many packages:

The following commands are useful for managing package source files and their installation when building LAMMPS via traditional make. Just type "make" in lammps/src to see a one-line summary.

These commands install/un-install sets of packages:

```
make yes-all                        # install all packages
make no-all                         # uninstall all packages
make yes-standard or make yes-std   # install standard packages
make no-standard or make no-std     # uninstall standard packages
make yes-user                       # install user packages
make no-user                        # uninstall user packages
make yes-lib                        # install packages that require extra libraries
make no-lib                         # uninstall packages that require extra libraries
make yes-ext                        # install packages that require external libraries
make no-ext                         # uninstall packages that require external␣
↪libraries
```

which install/un-install various sets of packages. Typing "make package" will list all the these commands.

Note: Installing or un-installing a package for the make based build process works by simply copying files back and forth between the main source directory src and the sub-directories with the package name (e.g. src/KSPACE, src/USER-ATC), so that the files are included or excluded when LAMMPS is built. Only source files in the src folder will be compiled.

The following make commands help manage files that exist in both the src directory and in package sub-directories. You do not normally need to use these commands unless you are editing LAMMPS files or are *installing a patch* downloaded from the LAMMPS web site.

Type "make package-status" or "make ps" to show which packages are currently installed. For those that are installed, it will list any files that are different in the src directory and package sub-directory.

Type "make package-installed" or "make pi" to show which packages are currently installed, without listing the status of packages that are not installed.

Type "make package-update" or "make pu" to overwrite src files with files from the package sub-directories if the package is installed. It should be used after a *patch has been applied*, since patches only update the files in the package sub-directory, but not the src files.

Type "make package-overwrite" to overwrite files in the package sub-directories with src files.

Type "make package-diff" to list all differences between pairs of files in both the source directory and the package directory.

3.7 Packages with extra build options

When building with some packages, additional steps may be required, in addition to:

```
$ cmake -D PKG_NAME=yes
```

or

```
$ make yes-name
```

as described on the *Build_package* doc page.

For a CMake build there may be additional optional or required variables to set. For a build with make, a provided library under the lammps/lib directory may need to be built first. Or an external library may need to exist on your system or be downloaded and built. You may need to tell LAMMPS where it is found on your system.

This is the list of packages that may require additional steps.

COMPRESS	*GPU*	*KIM*	*KOKKOS*	*LATTE*	*MESSAGE*
MSCG	*OPT*	*POEMS*	*PYTHON*	*VORONOI*	*USER-ADIOS*
USER-ATC	*USER-AWPMD*	*USER-COLVARS*	*USER-H5MD*	*USER-INTEL*	*USER-MOLFILE*
USER-NETCDF	*USER-PLUMED*	*USER-OMP*	*USER-QMMM*	*USER-QUIP*	*USER-SCAFACOS*
USER-SMD	*USER-VTK*				

3.7.1 COMPRESS package

To build with this package you must have the zlib compression library available on your system.

CMake build:

If CMake cannot find the library, you can set these variables:

```
-D ZLIB_INCLUDE_DIR=path     # path to zlib.h header file
-D ZLIB_LIBRARIES=path       # path to libz.a (.so) file
```

Traditional make:

If make cannot find the library, you can edit the file lib/compress/Makefile.lammps to specify the paths and library name.

3.7.2 GPU package

To build with this package, you must choose options for precision and which GPU hardware to build for.

CMake build:

```
-D GPU_API=value           # value = opencl (default) or cuda
-D GPU_PREC=value          # precision setting
                           # value = double or mixed (default) or single
-D OCL_TUNE=value          # hardware choice for GPU_API=opencl
                           # generic (default) or intel (Intel CPU) or fermi, kepler,␣
↪cypress (NVIDIA)
-D GPU_ARCH=value          # primary GPU hardware choice for GPU_API=cuda
                           # value = sm_XX, see below
                           # default is sm_30
-D CUDPP_OPT=value         # optimization setting for GPU_API=cuda
                           # enables CUDA Performance Primitives Optimizations
                           # value = yes (default) or no
-D CUDA_MPS_SUPPORT=value # enables some tweaks required to run with active nvidia-
↪cuda-mps daemon
                           # value = yes or no (default)
```

GPU_ARCH settings for different GPU hardware is as follows:

- sm_12 or sm_13 for GT200 (supported by CUDA 3.2 until CUDA 6.5)
- sm_20 or sm_21 for Fermi (supported by CUDA 3.2 until CUDA 7.5)
- sm_30 or sm_35 or sm_37 for Kepler (supported since CUDA 5)
- sm_50 or sm_52 for Maxwell (supported since CUDA 6)
- sm_60 or sm_61 for Pascal (supported since CUDA 8)
- sm_70 for Volta (supported since CUDA 9)
- sm_75 for Turing (supported since CUDA 10)

A more detailed list can be found, for example, at Wikipedia's CUDA article

CMake can detect which version of the CUDA toolkit is used and thus can include support for **all** major GPU architectures supported by this toolkit. Thus the GPU_ARCH setting is merely an optimization, to have code for the preferred GPU architecture directly included rather than having to wait for the JIT compiler of the CUDA driver to translate it.

Traditional make:

Before building LAMMPS, you must build the GPU library in lib/gpu. You can do this manually if you prefer; follow the instructions in lib/gpu/README. Note that the GPU library uses MPI calls, so you must use the same MPI library (or the STUBS library) settings as the main LAMMPS code. This also applies to the -DLAMMPS_BIGBIG, -DLAMMPS_SMALLBIG, or -DLAMMPS_SMALLSMALL settings in whichever Makefile you use.

You can also build the library in one step from the lammps/src dir, using a command like these, which simply invoke the lib/gpu/Install.py script with the specified args:

```
$ make lib-gpu               # print help message
$ make lib-gpu args="-b"     # build GPU library with default Makefile.linux
$ make lib-gpu args="-m xk7 -p single -o xk7.single"  # create new Makefile.xk7.
↪single, altered for single-precision
$ make lib-gpu args="-m mpi -a sm_60 -p mixed -b" # build GPU library with mixed␣
↪precision and P100 using other settings in Makefile.mpi
```

Note that this procedure starts with a Makefile.machine in lib/gpu, as specified by the "-m" switch. For your convenience, machine makefiles for "mpi" and "serial" are provided, which have the same settings as the corresponding machine makefiles in the main LAMMPS source folder. In addition you can alter 4 important settings in the Makefile.machine you start from via the corresponding -c, -a, -p, -e switches (as in the examples above), and also save a copy of the new Makefile if desired:

- CUDA_HOME = where NVIDIA CUDA software is installed on your system

- CUDA_ARCH = sm_XX, what GPU hardware you have, same as CMake GPU_ARCH above
- CUDA_PRECISION = precision (double, mixed, single)
- EXTRAMAKE = which Makefile.lammps.* file to copy to Makefile.lammps

The file Makefile.linux_multi is set up to include support for multiple GPU architectures as supported by the CUDA toolkit in use. This is done through using the "–gencode " flag, which can be used multiple times and thus support all GPU architectures supported by your CUDA compiler.

If the library build is successful, 3 files should be created: lib/gpu/libgpu.a, lib/gpu/nvc_get_devices, and lib/gpu/Makefile.lammps. The latter has settings that enable LAMMPS to link with CUDA libraries. If the settings in Makefile.lammps for your machine are not correct, the LAMMPS build will fail, and lib/gpu/Makefile.lammps may need to be edited.

Note: If you re-build the GPU library in lib/gpu, you should always un-install the GPU package in lammps/src, then re-install it and re-build LAMMPS. This is because the compilation of files in the GPU package uses the library settings from the lib/gpu/Makefile.machine used to build the GPU library.

3.7.3 KIM package

To build with this package, the KIM library with API v2 must be downloaded and built on your system. It must include the KIM models that you want to use with LAMMPS. If you want to use the *kim_query* command, you also need to have libcurl installed with the matching development headers and the curl-config tool.

See the Obtaining KIM Models web page to learn how to install a pre-build binary of the OpenKIM Repository of Models. See the list of all KIM models here: https://openkim.org/browse/models

(Also note that when downloading and installing from source the KIM API library with all its models, may take a long time (tens of minutes to hours) to build. Of course you only need to do that once.)

CMake build:

```
-D DOWNLOAD_KIM=value           # download OpenKIM API v2 for build, value = no␣
↪(default) or yes
-D LMP_DEBUG_CURL=value         # set libcurl verbose mode on/off, value = off␣
↪(default) or on
-D LMP_NO_SSL_CHECK=value       # tell libcurl to not verify the peer, value = no␣
↪(default) or yes
```

If DOWNLOAD_KIM is set, the KIM library will be downloaded and built inside the CMake build directory. If the KIM library is already on your system (in a location CMake cannot find it), set the PKG_CONFIG_PATH environment variable so that libkim-api can be found.

For using OpenKIM web queries in LAMMPS:

If LMP_DEBUG_CURL is set, the libcurl verbose mode will be on, and any libcurl calls within the KIM web query display a lot of information about libcurl operations. You hardly ever want this set in production use, you will almost always want this when you debug/report problems.

The libcurl performs peer SSL certificate verification by default. This verification is done using a CA certificate store that the SSL library can use to make sure the peer's server certificate is valid. If SSL reports an error ("certificate verify failed") during the handshake and thus refuses further communication with that server, you can set LMP_NO_SSL_CHECK. If LMP_NO_SSL_CHECK is set, libcurl does not verify the peer and connection succeeds regardless of the names in the certificate. This option is insecure. As an alternative, you can specify your own CA

cert path by setting the environment variable CURL_CA_BUNDLE to the path of your choice. A call to the KIM web query would get this value from the environmental variable.

Traditional make:

You can download and build the KIM library manually if you prefer; follow the instructions in lib/kim/README. You can also do it in one step from the lammps/src dir, using a command like these, which simply invoke the lib/kim/Install.py script with the specified args.

```
$ make lib-kim              # print help message
$ make lib-kim args="-b "   # (re-)install KIM API lib with only example models
$ make lib-kim args="-b -a Glue_Ercolessi_Adams_Al__MO_324507536345_001"  # ditto␣
↪plus one model
$ make lib-kim args="-b -a everything"     # install KIM API lib with all models
$ make lib-kim args="-n -a EAM_Dynamo_Ackland_W__MO_141627196590_002"       # add one␣
↪model or model driver
$ make lib-kim args="-p /usr/local" # use an existing KIM API installation at the␣
↪provided location
$ make lib-kim args="-p /usr/local -a EAM_Dynamo_Ackland_W__MO_141627196590_002" #␣
↪ditto but add one model or driver
```

Settings for OpenKIM web queries discussed above need to be applied by adding them to the LMP_INC variable through editing the Makefile.machine you are using. For example:

```
LMP_INC =       -DLMP_NO_SSL_CHECK
```

3.7.4 KOKKOS package

To build with this package, you must choose which hardware you want to build for, either CPUs (multi-threading via OpenMP) or KNLs (OpenMP) or GPUs (NVIDIA Cuda).

For a CMake or make build, these are the possible choices for the KOKKOS_ARCH settings described below. Note that for CMake, these are really Kokkos variables, not LAMMPS variables. Hence you must use case-sensitive values, e.g. BDW, not bdw.

- AMDAVX = AMD 64-bit x86 CPUs
- EPYC = AMD EPYC Zen class CPUs
- ARMv80 = ARMv8.0 Compatible CPU
- ARMv81 = ARMv8.1 Compatible CPU
- ARMv8-ThunderX = ARMv8 Cavium ThunderX CPU
- ARMv8-TX2 = ARMv8 Cavium ThunderX2 CPU
- WSM = Intel Westmere CPUs
- SNB = Intel Sandy/Ivy Bridge CPUs
- HSW = Intel Haswell CPUs
- BDW = Intel Broadwell Xeon E-class CPUs
- SKX = Intel Sky Lake Xeon E-class HPC CPUs (AVX512)
- KNC = Intel Knights Corner Xeon Phi
- KNL = Intel Knights Landing Xeon Phi

- BGQ = IBM Blue Gene/Q CPUs
- Power7 = IBM POWER8 CPUs
- Power8 = IBM POWER8 CPUs
- Power9 = IBM POWER9 CPUs
- Kepler = NVIDIA Kepler default (generation CC 3.5)
- Kepler30 = NVIDIA Kepler generation CC 3.0
- Kepler32 = NVIDIA Kepler generation CC 3.2
- Kepler35 = NVIDIA Kepler generation CC 3.5
- Kepler37 = NVIDIA Kepler generation CC 3.7
- Maxwell = NVIDIA Maxwell default (generation CC 5.0)
- Maxwell50 = NVIDIA Maxwell generation CC 5.0
- Maxwell52 = NVIDIA Maxwell generation CC 5.2
- Maxwell53 = NVIDIA Maxwell generation CC 5.3
- Pascal60 = NVIDIA Pascal generation CC 6.0
- Pascal61 = NVIDIA Pascal generation CC 6.1
- Volta70 = NVIDIA Volta generation CC 7.0
- Volta72 = NVIDIA Volta generation CC 7.2
- Turing75 = NVIDIA Turing generation CC 7.5

CMake build:

For multicore CPUs using OpenMP, set these 2 variables.

```
-D KOKKOS_ARCH=archCPU          # archCPU = CPU from list above
-D KOKKOS_ENABLE_OPENMP=yes
```

For Intel KNLs using OpenMP, set these 2 variables:

```
-D KOKKOS_ARCH=KNL
-D KOKKOS_ENABLE_OPENMP=yes
```

For NVIDIA GPUs using CUDA, set these 4 variables:

```
-D KOKKOS_ARCH="archCPU;archGPU"    # archCPU = CPU from list above that is hosting␣
↪the GPU
                                    # archGPU = GPU from list above
-D KOKKOS_ENABLE_CUDA=yes
-D KOKKOS_ENABLE_OPENMP=yes
-D CMAKE_CXX_COMPILER=wrapper       # wrapper = full path to Cuda nvcc wrapper
```

The wrapper value is the Cuda nvcc compiler wrapper provided in the Kokkos library: lib/kokkos/bin/nvcc_wrapper. The setting should include the full path name to the wrapper, e.g.

```
-D CMAKE_CXX_COMPILER=/home/username/lammps/lib/kokkos/bin/nvcc_wrapper
```

Traditional make:

Choose which hardware to support in Makefile.machine via KOKKOS_DEVICES and KOKKOS_ARCH settings. See the src/MAKE/OPTIONS/Makefile.kokkos* files for examples.

For multicore CPUs using OpenMP:

```
KOKKOS_DEVICES = OpenMP
KOKKOS_ARCH = archCPU       # archCPU = CPU from list above
```

For Intel KNLs using OpenMP:

```
KOKKOS_DEVICES = OpenMP
KOKKOS_ARCH = KNL
```

For NVIDIA GPUs using CUDA:

```
KOKKOS_DEVICES = Cuda
KOKKOS_ARCH = archCPU,archGPU     # archCPU = CPU from list above that is hosting the␣
↪GPU
                                  # archGPU = GPU from list above
FFT_INC = -DFFT_CUFFT             # enable use of cuFFT (optional)
FFT_LIB = -lcufft                 # link to cuFFT library
```

For GPUs, you also need the following 2 lines in your Makefile.machine before the CC line is defined, in this case for use with OpenMPI mpicxx. The 2 lines define a nvcc wrapper compiler, which will use nvcc for compiling CUDA files and use a C++ compiler for non-Kokkos, non-CUDA files.

```
KOKKOS_ABSOLUTE_PATH = $(shell cd $(KOKKOS_PATH); pwd)
export OMPI_CXX = $(KOKKOS_ABSOLUTE_PATH)/config/nvcc_wrapper
CC =            mpicxx
```

3.7.5 LATTE package

To build with this package, you must download and build the LATTE library.

CMake build:

```
-D DOWNLOAD_LATTE=value     # download LATTE for build, value = no (default) or yes
-D LATTE_LIBRARY=path       # LATTE library file (only needed if a custom location)
```

If DOWNLOAD_LATTE is set, the LATTE library will be downloaded and built inside the CMake build directory. If the LATTE library is already on your system (in a location CMake cannot find it), LATTE_LIBRARY is the filename (plus path) of the LATTE library file, not the directory the library file is in.

Traditional make:

You can download and build the LATTE library manually if you prefer; follow the instructions in lib/latte/README. You can also do it in one step from the lammps/src dir, using a command like these, which simply invokes the lib/latte/Install.py script with the specified args:

```
$ make lib-latte                          # print help message
$ make lib-latte args="-b"                # download and build in lib/latte/LATTE-
↪master
$ make lib-latte args="-p $HOME/latte"    # use existing LATTE installation in $HOME/
↪latte
$ make lib-latte args="-b -m gfortran"    # download and build in lib/latte and
                                         #   copy Makefile.lammps.gfortran to␣
↪Makefile.lammps
```

Note that 3 symbolic (soft) links, "includelink" and "liblink" and "filelink.o", are created in lib/latte to point into the LATTE home dir. When LAMMPS itself is built it will use these links. You should also check that the Makefile.lammps file you create is appropriate for the compiler you use on your system to build LATTE.

3.7.6 MESSAGE package

This package can optionally include support for messaging via sockets, using the open-source ZeroMQ library, which must be installed on your system.

CMake build:

```
-D MESSAGE_ZMQ=value     # build with ZeroMQ support, value = no (default) or yes
-D ZMQ_LIBRARY=path      # ZMQ library file (only needed if a custom location)
-D ZMQ_INCLUDE_DIR=path # ZMQ include directory (only needed if a custom location)
```

Traditional make:

Before building LAMMPS, you must build the CSlib library in lib/message. You can build the CSlib library manually if you prefer; follow the instructions in lib/message/README. You can also do it in one step from the lammps/src dir, using a command like these, which simply invoke the lib/message/Install.py script with the specified args:

```
$ make lib-message                # print help message
$ make lib-message args="-m -z"   # build with MPI and socket (ZMQ) support
$ make lib-message args="-s"      # build as serial lib with no ZMQ support
```

The build should produce two files: lib/message/cslib/src/libmessage.a and lib/message/Makefile.lammps. The latter is copied from an existing Makefile.lammps.* and has settings to link with the ZeroMQ library if requested in the build.

3.7.7 MSCG package

To build with this package, you must download and build the MS-CG library. Building the MS-CG library and using it from LAMMPS requires a C++11 compatible compiler and that the GSL (GNU Scientific Library) headers and libraries are installed on your machine. See the lib/mscg/README and MSCG/Install files for more details.

CMake build:

```
-D DOWNLOAD_MSCG=value     # download MSCG for build, value = no (default) or yes
-D MSCG_LIBRARY=path       # MSCG library file (only needed if a custom location)
-D MSCG_INCLUDE_DIR=path   # MSCG include directory (only needed if a custom location)
```

If DOWNLOAD_MSCG is set, the MSCG library will be downloaded and built inside the CMake build directory. If the MSCG library is already on your system (in a location CMake cannot find it), MSCG_LIBRARY is the filename (plus path) of the MSCG library file, not the directory the library file is in. MSCG_INCLUDE_DIR is the directory the MSCG include file is in.

Traditional make:

You can download and build the MS-CG library manually if you prefer; follow the instructions in lib/mscg/README. You can also do it in one step from the lammps/src dir, using a command like these, which simply invoke the lib/mscg/Install.py script with the specified args:

```
$ make lib-mscg              # print help message
$ make lib-mscg args="-b -m serial"   # download and build in lib/mscg/MSCG-release-
↪master
                                      # with the settings compatible with "make serial"
$ make lib-mscg args="-b -m mpi"      # download and build in lib/mscg/MSCG-release-
↪master
                                      # with the settings compatible with "make mpi"
$ make lib-mscg args="-p /usr/local/mscg-release" # use the existing MS-CG␣
↪installation in /usr/local/mscg-release
```

Note that 2 symbolic (soft) links, "includelink" and "liblink", will be created in lib/mscg to point to the MS-CG src/installation dir. When LAMMPS is built in src it will use these links. You should not need to edit the lib/mscg/Makefile.lammps file.

3.7.8 OPT package

CMake build:

No additional settings are needed besides "-D PKG_OPT=yes".

Traditional make:

The compile flag "-restrict" must be used to build LAMMPS with the OPT package when using Intel compilers. It should be added to the CCFLAGS line of your Makefile.machine. See src/MAKE/OPTIONS/Makefile.opt for an example.

3.7.9 POEMS package

CMake build:

No additional settings are needed besides "-D PKG_OPT=yes".

Traditional make:

Before building LAMMPS, you must build the POEMS library in lib/poems. You can do this manually if you prefer; follow the instructions in lib/poems/README. You can also do it in one step from the lammps/src dir, using a command like these, which simply invoke the lib/poems/Install.py script with the specified args:

```
$ make lib-poems                   # print help message
$ make lib-poems args="-m serial"  # build with GNU g++ compiler (settings as with
↪"make serial")
$ make lib-poems args="-m mpi"     # build with default MPI C++ compiler (settings as␣
↪with "make mpi")
$ make lib-poems args="-m icc"     # build with Intel icc compiler
```

The build should produce two files: lib/poems/libpoems.a and lib/poems/Makefile.lammps. The latter is copied from an existing Makefile.lammps.* and has settings needed to build LAMMPS with the POEMS library (though typically the settings are just blank). If necessary, you can edit/create a new lib/poems/Makefile.machine file for your system, which should define an EXTRAMAKE variable to specify a corresponding Makefile.lammps.machine file.

3.7.10 PYTHON package

Building with the PYTHON package requires you have a Python shared library available on your system, which needs to be a Python 2 version, 2.6 or later. Python 3 is not yet supported. See lib/python/README for more details.

CMake build:

```
-D PYTHON_EXECUTABLE=path    # path to Python executable to use
```

Without this setting, CMake will guess the default Python on your system. To use a different Python version, you can either create a virtualenv, activate it and then run cmake. Or you can set the PYTHON_EXECUTABLE variable to specify which Python interpreter should be used. Note note that you will also need to have the development headers installed for this version, e.g. python2-devel.

Traditional make:

The build uses the lib/python/Makefile.lammps file in the compile/link process to find Python. You should only need to create a new Makefile.lammps.* file (and copy it to Makefile.lammps) if the LAMMPS build fails.

3.7.11 VORONOI package

To build with this package, you must download and build the Voro++ library.

CMake build:

```
-D DOWNLOAD_VORO=value     # download Voro++ for build, value = no (default) or yes
-D VORO_LIBRARY=path       # Voro++ library file (only needed if at custom location)
-D VORO_INCLUDE_DIR=path   # Voro++ include directory (only needed if at custom␣
↪location)
```

If DOWNLOAD_VORO is set, the Voro++ library will be downloaded and built inside the CMake build directory. If the Voro++ library is already on your system (in a location CMake cannot find it), VORO_LIBRARY is the filename (plus path) of the Voro++ library file, not the directory the library file is in. VORO_INCLUDE_DIR is the directory the Voro++ include file is in.

Traditional make:

You can download and build the Voro++ library manually if you prefer; follow the instructions in lib/voronoi/README. You can also do it in one step from the lammps/src dir, using a command like these, which simply invoke the lib/voronoi/Install.py script with the specified args:

```
$ make lib-voronoi                          # print help message
$ make lib-voronoi args="-b"                # download and build the default version␣
↪in lib/voronoi/voro++-<version>
$ make lib-voronoi args="-p $HOME/voro++"   # use existing Voro++ installation in
↪$HOME/voro++
$ make lib-voronoi args="-b -v voro++0.4.6" # download and build the 0.4.6 version in␣
↪lib/voronoi/voro++-0.4.6
```

Note that 2 symbolic (soft) links, “includelink” and “liblink”, are created in lib/voronoi to point to the Voro++ src dir. When LAMMPS builds in src it will use these links. You should not need to edit the lib/voronoi/Makefile.lammps file.

3.7.12 USER-ADIOS package

The USER-ADIOS package requires the ADIOS I/O library, version 2.3.1 or newer. Make sure that you have ADIOS built either with or without MPI to match if you build LAMMPS with or without MPI. ADIOS compilation settings for LAMMPS are automatically detected, if the PATH and LD_LIBRARY_PATH environment variables have been updated for the local ADIOS installation and the instructions below are followed for the respective build systems.

CMake build:

```
-D ADIOS2_DIR=path        # path is where ADIOS 2.x is installed
-D PKG_USER-ADIOS=yes
```

Traditional make:

Turn on the USER-ADIOS package before building LAMMPS. If the ADIOS 2.x software is installed in PATH, there is nothing else to do:

```
$ make yes-user-adios
```

otherwise, set ADIOS2_DIR environment variable when turning on the package:

```
$ ADIOS2_DIR=path make yes-user-adios   # path is where ADIOS 2.x is installed
```

3.7.13 USER-ATC package

The USER-ATC package requires the MANYBODY package also be installed.

CMake build:

No additional settings are needed besides "-D PKG_USER-ATC=yes" and "-D PKG_MANYBODY=yes".

Traditional make:

Before building LAMMPS, you must build the ATC library in lib/atc. You can do this manually if you prefer; follow the instructions in lib/atc/README. You can also do it in one step from the lammps/src dir, using a command like these, which simply invoke the lib/atc/Install.py script with the specified args:

```
$ make lib-atc                      # print help message
$ make lib-atc args="-m serial"     # build with GNU g++ compiler and MPI STUBS␣
↪(settings as with "make serial")
$ make lib-atc args="-m mpi"        # build with default MPI compiler (settings as␣
↪with "make mpi")
$ make lib-atc args="-m icc"        # build with Intel icc compiler
```

The build should produce two files: lib/atc/libatc.a and lib/atc/Makefile.lammps. The latter is copied from an existing Makefile.lammps.* and has settings needed to build LAMMPS with the ATC library. If necessary, you can edit/create a new lib/atc/Makefile.machine file for your system, which should define an EXTRAMAKE variable to specify a corresponding Makefile.lammps.machine file.

Note that the Makefile.lammps file has settings for the BLAS and LAPACK linear algebra libraries. As explained in lib/atc/README these can either exist on your system, or you can use the files provided in lib/linalg. In the latter case you also need to build the library in lib/linalg with a command like these:

```
$ make lib-linalg                      # print help message
$ make lib-linalg args="-m serial"     # build with GNU Fortran compiler (settings as␣
↪with "make serial")
$ make lib-linalg args="-m mpi"        # build with default MPI Fortran compiler␣
↪(settings as with "make mpi")
$ make lib-linalg args="-m gfortran"   # build with GNU Fortran compiler
```

3.7.14 USER-AWPMD package

CMake build:

No additional settings are needed besides "-D PKG_USER-AQPMD=yes".

Traditional make:

Before building LAMMPS, you must build the AWPMD library in lib/awpmd. You can do this manually if you prefer; follow the instructions in lib/awpmd/README. You can also do it in one step from the lammps/src dir, using a command like these, which simply invoke the lib/awpmd/Install.py script with the specified args:

```
$ make lib-awpmd                    # print help message
$ make lib-awpmd args="-m serial"   # build with GNU g++ compiler and MPI STUBS␣
↪(settings as with "make serial")
$ make lib-awpmd args="-m mpi"      # build with default MPI compiler (settings as␣
↪with "make mpi")
$ make lib-awpmd args="-m icc"      # build with Intel icc compiler
```

The build should produce two files: lib/awpmd/libawpmd.a and lib/awpmd/Makefile.lammps. The latter is copied from an existing Makefile.lammps.* and has settings needed to build LAMMPS with the AWPMD library. If necessary, you can edit/create a new lib/awpmd/Makefile.machine file for your system, which should define an EXTRAMAKE variable to specify a corresponding Makefile.lammps.machine file.

Note that the Makefile.lammps file has settings for the BLAS and LAPACK linear algebra libraries. As explained in lib/awpmd/README these can either exist on your system, or you can use the files provided in lib/linalg. In the latter case you also need to build the library in lib/linalg with a command like these:

```
$ make lib-linalg                      # print help message
$ make lib-linalg args="-m serial"     # build with GNU Fortran compiler (settings as␣
↪with "make serial")
$ make lib-linalg args="-m mpi"        # build with default MPI Fortran compiler␣
↪(settings as with "make mpi")
$ make lib-linalg args="-m gfortran"   # build with GNU Fortran compiler
```

3.7.15 USER-COLVARS package

This package includes into the LAMMPS distribution the Colvars library, which can be built for the most part with all major versions of the C++ language.

A few of the most recent features require C++11 support. In particular, the library is optionally built together with the Lepton library, a copy of which is also included in the LAMMPS distribution. Lepton implements the customFunction feature, and requires C++11 support.

See here for a detailed list of C++11-only features.

CMake build:

This is the recommended build recipe: no additional settings are normally needed besides "-D PKG_USER-COLVARS=yes".

Building and linking of Lepton (or other C++11-only features) is enabled automatically when compilation is carried out with C++11 support, and disabled otherwise. Optionally, Lepton build may be manually controlled with the flag "-D COLVARS_LEPTON=yes|no".

Traditional make:

Before building LAMMPS, one must build the Colvars library in lib/colvars.

This can be done manually in the same folder by using or adapting one of the provided Makefiles: for example, Makefile.g++ for the GNU compiler.

In general, it is safer to use build setting consistent with the rest of LAMMPS. This is best carried out from the LAMMPS src directory using a command like these, which simply invoke the lib/colvars/Install.py script with the specified args:

```
$ make lib-colvars                      # print help message
$ make lib-colvars args="-m serial"     # build with GNU g++ compiler (settings as␣
↪with "make serial")
$ make lib-colvars args="-m mpi"        # build with default MPI compiler (settings␣
↪as with "make mpi")
$ make lib-colvars args="-m g++-debug"  # build with GNU g++ compiler and colvars␣
↪debugging enabled
```

The "machine" argument of the "-m" flag is used to find a Makefile.machine to use as build recipe. If it does not already exist in lib/colvars, it will be auto-generated by using compiler flags consistent with those parsed from the core LAMMPS makefiles.

Optional flags may be specified as environment variables:

```
$ COLVARS_DEBUG=yes make lib-colvars args="-m machine"  # Build with debug code (much␣
↪slower)
$ COLVARS_LEPTON=no make lib-colvars args="-m machine"  # Build without Lepton␣
↪(included otherwise)
```

The build should produce two files: the library lib/colvars/libcolvars.a (which also includes Lepton objects if enabled) and the specification file lib/colvars/Makefile.lammps. The latter is auto-generated, and normally does not need to be edited.

3.7.16 USER-PLUMED package

Before building LAMMPS with this package, you must first build PLUMED. PLUMED can be built as part of the LAMMPS build or installed separately from LAMMPS using the generic plumed installation instructions. The USER-PLUMED package has been tested to work with Plumed versions 2.4.x, 2.5.x, and 2.6.x and will error out, when trying to run calculations with a different version of the Plumed kernel.

PLUMED can be linked into MD codes in three different modes: static, shared, and runtime. With the "static" mode, all the code that PLUMED requires is linked statically into LAMMPS. LAMMPS is then fully independent from the PLUMED installation, but you have to rebuild/relink it in order to update the PLUMED code inside it. With the "shared" linkage mode, LAMMPS is linked to a shared library that contains the PLUMED code. This library should preferably be installed in a globally accessible location. When PLUMED is linked in this way the same library can be used by multiple MD packages. Furthermore, the PLUMED library LAMMPS uses can be updated without the need for a recompile of LAMMPS for as long as the shared PLUMED library is ABI-compatible.

The third linkage mode is "runtime" which allows the user to specify which PLUMED kernel should be used at runtime by using the PLUMED_KERNEL environment variable. This variable should point to the location of the libplumedKernel.so dynamical shared object, which is then loaded at runtime. This mode of linking is particularly convenient for doing PLUMED development and comparing multiple PLUMED versions as these sorts of comparisons can be done without recompiling the hosting MD code. All three linkage modes are supported by LAMMPS on selected operating systems (e.g. Linux) and using either CMake or traditional make build. The "static" mode should be the most portable, while the "runtime" mode support in LAMMPS makes the most assumptions about operating system and compiler environment. If one mode does not work, try a different one, switch to a different build system, consider a global PLUMED installation or consider downloading PLUMED during the LAMMPS build.

CMake build:

When the "-D PKG_USER-PLUMED" flag is included in the cmake command you must ensure that GSL is installed in locations that are specified in your environment. There are then two additional commands that control the manner in which PLUMED is obtained and linked into LAMMPS.

```
-D DOWNLOAD_PLUMED=value    # download PLUMED for build, value = no (default) or yes
-D PLUMED_MODE=value        # Linkage mode for PLUMED, value = static (default),␣
↪shared, or runtime
```

If DOWNLOAD_PLUMED is set to "yes", the PLUMED library will be downloaded (the version of PLUMED that will be downloaded is hard-coded to a vetted version of PLUMED, usually a recent stable release version) and built inside the CMake build directory. If DOWNLOAD_PLUMED is set to "no" (the default), CMake will try to detect and link to an installed version of PLUMED. For this to work, the PLUMED library has to be installed into a location where the pkg-config tool can find it or the PKG_CONFIG_PATH environment variable has to be set up accordingly. PLUMED should be installed in such a location if you compile it using the default make; make install commands.

The PLUMED_MODE setting determines the linkage mode for the PLUMED library. The allowed values for this flag are "static" (default), "shared", or "runtime". For a discussion of PLUMED linkage modes, please see above. When DOWNLOAD_PLUMED is enabled the static linkage mode is recommended.

Traditional make:

PLUMED needs to be installed before the USER-PLUMED package is installed so that LAMMPS can find the right settings when compiling and linking the LAMMPS executable. You can either download and build PLUMED inside the LAMMPS plumed library folder or use a previously installed PLUMED library and point LAMMPS to its location. You also have to choose the linkage mode: "static" (default), "shared" or "runtime". For a discussion of PLUMED linkage modes, please see above.

Download/compilation/configuration of the plumed library can be done from the src folder through the following make args:

```
$ make lib-plumed                          # print help message
$ make lib-plumed args="-b"                # download and build PLUMED in lib/plumed/
↪plumed2
$ make lib-plumed args="-p $HOME/.local"   # use existing PLUMED installation in $HOME/
↪.local
$ make lib-plumed args="-p /usr/local -m shared"  # use existing PLUMED installation␣
↪in
                                                  # /usr/local and use shared linkage␣
↪mode
```

Note that 2 symbolic (soft) links, "includelink" and "liblink" are created in lib/plumed that point to the location of the PLUMED build to use. A new file lib/plumed/Makefile.lammps is also created with settings suitable for LAMMPS to compile and link PLUMED using the desired linkage mode. After this step is completed, you can install the USER-PLUMED package and compile LAMMPS in the usual manner:

```
$ make yes-user-plumed
$ make machine
```

Once this compilation completes you should be able to run LAMMPS in the usual way. For shared linkage mode, libplumed.so must be found by the LAMMPS executable, which on many operating systems means, you have to set the LD_LIBRARY_PATH environment variable accordingly.

Support for the different linkage modes in LAMMPS varies for different operating systems, using the static linkage is expected to be the most portable, and thus set to be the default.

If you want to change the linkage mode, you have to re-run "make lib-plumed" with the desired settings **and** do a re-install if the USER-PLUMED package with "make yes-user-plumed" to update the required makefile settings with the changes in the lib/plumed folder.

3.7.17 USER-H5MD package

To build with this package you must have the HDF5 software package installed on your system, which should include the h5cc compiler and the HDF5 library.

CMake build:

No additional settings are needed besides "-D PKG_USER-H5MD=yes".

This should auto-detect the H5MD library on your system. Several advanced CMake H5MD options exist if you need to specify where it is installed. Use the ccmake (terminal window) or cmake-gui (graphical) tools to see these options and set them interactively from their user interfaces.

Traditional make:

Before building LAMMPS, you must build the CH5MD library in lib/h5md. You can do this manually if you prefer; follow the instructions in lib/h5md/README. You can also do it in one step from the lammps/src dir, using a command like these, which simply invoke the lib/h5md/Install.py script with the specified args:

```
$ make lib-h5md                     # print help message
$ make lib-h5md args="-m h5cc"      # build with h5cc compiler
```

The build should produce two files: lib/h5md/libch5md.a and lib/h5md/Makefile.lammps. The latter is copied from an existing Makefile.lammps.* and has settings needed to build LAMMPS with the system HDF5 library. If necessary, you can edit/create a new lib/h5md/Makefile.machine file for your system, which should define an EXTRAMAKE variable to specify a corresponding Makefile.lammps.machine file.

3.7.18 USER-INTEL package

To build with this package, you must choose which hardware you want to build for, either x86 CPUs or Intel KNLs in offload mode. You should also typically *install the USER-OMP package*, as it can be used in tandem with the USER-INTEL package to good effect, as explained on the *Speed intel* doc page.

CMake build:

```
-D INTEL_ARCH=value      # value = cpu (default) or knl
-D INTEL_LRT_MODE=value # value = threads, none, or c++11
```

In Long-range thread mode (LRT) a modified verlet style is used, that operates the Kspace calculation in a separate thread concurrently to other calculations. This has to be enabled in the *package intel* command at runtime. With the setting "threads" it used the pthreads library, while c++11 will use the built-in thread support of C++11 compilers. The option "none" skips compilation of this feature. The default is to use "threads" if pthreads is available and otherwise "none".

Best performance is achieved with Intel hardware, Intel compilers, as well as the Intel TBB and MKL libraries. However, the code also compiles, links, and runs with other compilers and without TBB and MKL.

Traditional make:

Choose which hardware to compile for in Makefile.machine via the following settings. See src/MAKE/OPTIONS/Makefile.intel_cpu* and Makefile.knl files for examples. and src/USER-INTEL/README for additional information.

For CPUs:

```
OPTFLAGS =      -xHost -O2 -fp-model fast=2 -no-prec-div -qoverride-limits -qopt-zmm-
↪usage=high
CCFLAGS =       -g -qopenmp -DLAMMPS_MEMALIGN=64 -no-offload -fno-alias -ansi-alias -
↪restrict $(OPTFLAGS)
LINKFLAGS =     -g -qopenmp $(OPTFLAGS)
LIB =           -ltbbmalloc
```

For KNLs:

```
OPTFLAGS =      -xMIC-AVX512 -O2 -fp-model fast=2 -no-prec-div -qoverride-limits
CCFLAGS =       -g -qopenmp -DLAMMPS_MEMALIGN=64 -no-offload -fno-alias -ansi-alias -
↪restrict $(OPTFLAGS)
LINKFLAGS =     -g -qopenmp $(OPTFLAGS)
LIB =           -ltbbmalloc
```

3.7.19 USER-MOLFILE package

CMake build:

```
-D MOLFILE_INCLUDE_DIRS=path   # (optional) path where VMD molfile plugin headers are␣
↪installed
-D PKG_USER-MOLFILE=yes
```

Using "-D PKG_USER-MOLFILE=yes" enables the package, and setting "-D MOLFILE_INCLUDE DIRS" allows to provide a custom location for the molfile plugin header files. These should match the ABI of the plugin files used, and thus one typically sets them to include folder of the local VMD installation in use. LAMMPS ships with a couple of default header files that correspond to a popular VMD version, usually the latest release.

Traditional make:

The lib/molfile/Makefile.lammps file has a setting for a dynamic loading library libdl.a that is typically present on all systems. It is required for LAMMPS to link with this package. If the setting is not valid for your system, you will need to edit the Makefile.lammps file. See lib/molfile/README and lib/molfile/Makefile.lammps for details. It is also possible to configure a different folder with the VMD molfile plugin header files. LAMMPS ships with a couple of default headers, but these are not compatible with all VMD versions, so it is often best to change this setting to the location of the same include files of the local VMD installation in use.

3.7.20 USER-NETCDF package

To build with this package you must have the NetCDF library installed on your system.

CMake build:

No additional settings are needed besides "-D PKG_USER-NETCDF=yes".

This should auto-detect the NETCDF library if it is installed on your system at standard locations. Several advanced CMake NETCDF options exist if you need to specify where it was installed. Use the ccmake (terminal window) or cmake-gui (graphical) tools to see these options and set them interactively from their user interfaces.

Traditional make:

The lib/netcdf/Makefile.lammps file has settings for NetCDF include and library files which LAMMPS needs to build with this package. If the settings are not valid for your system, you will need to edit the Makefile.lammps file. See lib/netcdf/README for details.

3.7.21 USER-OMP package

CMake build:

No additional settings are required besides "-D PKG_USER-OMP=yes". If CMake detects OpenMP support, the USER-OMP code will be compiled with multi-threading support enabled, otherwise as optimized serial code.

Traditional make:

To enable multi-threading support in the USER-OMP package (and other styles supporting OpenMP) the following compile and link flags must be added to your Makefile.machine file. See src/MAKE/OPTIONS/Makefile.omp for an example.

```
CCFLAGS: -fopenmp               # for GNU and Clang Compilers
CCFLAGS: -qopenmp -restrict     # for Intel compilers on Linux
LINKFLAGS: -fopenmp             # for GNU and Clang Compilers
LINKFLAGS: -qopenmp             # for Intel compilers on Linux
```

For other platforms and compilers, please consult the documentation about OpenMP support for your compiler. Please see the note about how to address compatibility *issues with the 'default(none)' directive* of some compilers.

3.7.22 USER-QMMM package

For using LAMMPS to do QM/MM simulations via the USER-QMMM package you need to build LAMMPS as a library. A LAMMPS executable with fix qmmm included can be built, but will not be able to do a QM/MM simulation on as such. You must also build a QM code - currently only Quantum ESPRESSO (QE) is supported - and create a new executable which links LAMMPS and the QM code together. Details are given in the lib/qmmm/README file. It is also recommended to read the instructions for *linking with LAMMPS as a library* for background information. This requires compatible Quantum Espresso and LAMMPS versions. The current interface and makefiles have last been verified to work in February 2020 with Quantum Espresso versions 6.3 to 6.5.

CMake build:

When using CMake, building a LAMMPS library is required and it is recommended to build a shared library, since any libraries built from the sources in the *lib* folder (including the essential libqmmm.a) are not included in the static LAMMPS library and (currently) not installed, while their code is included in the shared LAMMPS library. Thus a typical command line to configure building LAMMPS for USER-QMMM would be:

```
cmake -C ../cmake/presets/minimal.cmake -D PKG_USER-QMMM=yes \
        -D BUILD_LIB=yes -DBUILD_SHARED_LIBS=yes ../cmake
```

After completing the LAMMPS build and also configuring and compiling Quantum ESPRESSO with external library support (via "make couple"), go back to the lib/qmmm folder and follow the instructions on the README file to build the combined LAMMPS/QE QM/MM executable (pwqmmm.x) in the lib/qmmm folder. You need to make certain, that

Traditional make:

Before building LAMMPS, you must build the QMMM library in lib/qmmm. You can do this manually if you prefer; follow the first two steps explained in lib/qmmm/README. You can also do it in one step from the lammps/src dir, using a command like these, which simply invoke the lib/qmmm/Install.py script with the specified args:

```
$ make lib-qmmm                      # print help message
$ make lib-qmmm args="-m serial"     # build with GNU Fortran compiler (settings as␣
↪in "make serial")
$ make lib-qmmm args="-m mpi"        # build with default MPI compiler (settings as␣
↪in "make mpi")
$ make lib-qmmm args="-m gfortran"   # build with GNU Fortran compiler
```

The build should produce two files: lib/qmmm/libqmmm.a and lib/qmmm/Makefile.lammps. The latter is copied from an existing Makefile.lammps.* and has settings needed to build LAMMPS with the QMMM library (though typically the settings are just blank). If necessary, you can edit/create a new lib/qmmm/Makefile.machine file for your system, which should define an EXTRAMAKE variable to specify a corresponding Makefile.lammps.machine file.

You can then install QMMM package and build LAMMPS in the usual manner. After completing the LAMMPS build and compiling Quantum ESPRESSO with external library support (via "make couple"), go back to the lib/qmmm folder and follow the instructions in the README file to build the combined LAMMPS/QE QM/MM executable (pwqmmm.x) in the lib/qmmm folder.

3.7.23 USER-QUIP package

To build with this package, you must download and build the QUIP library. It can be obtained from GitHub. For support of GAP potentials, additional files with specific licensing conditions need to be downloaded and configured. See step 1 and step 1.1 in the lib/quip/README file for details on how to do this.

CMake build:

```
-D QUIP_LIBRARY=path      # path to libquip.a (only needed if a custom location)
```

CMake will not download and build the QUIP library. But once you have done that, a CMake build of LAMMPS with "-D PKG_USER-QUIP=yes" should work. Set QUIP_LIBRARY if CMake cannot find the QUIP library.

Traditional make:

The download/build procedure for the QUIP library, described in lib/quip/README file requires setting two environment variables, QUIP_ROOT and QUIP_ARCH. These are accessed by the lib/quip/Makefile.lammps file which is used when you compile and link LAMMPS with this package. You should only need to edit Makefile.lammps if the LAMMPS build can not use its settings to successfully build on your system.

3.7.24 USER-SCAFACOS package

To build with this package, you must download and build the ScaFaCoS Coulomb solver library

CMake build:

```
-D DOWNLOAD_SCAFACOS=value     # download ScaFaCoS for build, value = no (default) or␣
↪yes
-D SCAFACOS_LIBRARY=path       # ScaFaCos library file (only needed if at custom␣
↪location)
-D SCAFACOS_INCLUDE_DIR=path   # ScaFaCoS include directory (only needed if at custom␣
↪location)
```

If DOWNLOAD_SCAFACOS is set, the ScaFaCoS library will be downloaded and built inside the CMake build directory. If the ScaFaCoS library is already on your system (in a location CMake cannot find it), SCAFACOS_LIBRARY is the filename (plus path) of the ScaFaCoS library file, not the directory the library file is in. SCAFACOS_INCLUDE_DIR is the directory the ScaFaCoS include file is in.

Traditional make:

You can download and build the ScaFaCoS library manually if you prefer; follow the instructions in lib/scafacos/README. You can also do it in one step from the lammps/src dir, using a command like these, which simply invoke the lib/scafacos/Install.py script with the specified args:

make lib-scafacos # print help message make lib-scafacos args="-b" # download and build in lib/scafacos/scafacos-<version> make lib-scafacos args="-p $HOME/scafacos # use existing ScaFaCoS installation in $HOME/scafacos

Note that 2 symbolic (soft) links, "includelink" and "liblink", are created in lib/scafacos to point to the ScaFaCoS src dir. When LAMMPS builds in src it will use these links. You should not need to edit the lib/scafacos/Makefile.lammps file.

3.7.25 USER-SMD package

To build with this package, you must download the Eigen3 library. Eigen3 is a template library, so you do not need to build it.

CMake build:

```
-D DOWNLOAD_EIGEN3             # download Eigen3, value = no (default) or yes
-D EIGEN3_INCLUDE_DIR=path     # path to Eigen library (only needed if a custom␣
↪location)
```

If DOWNLOAD_EIGEN3 is set, the Eigen3 library will be downloaded and inside the CMake build directory. If the Eigen3 library is already on your system (in a location CMake cannot find it), EIGEN3_INCLUDE_DIR is the directory the Eigen3++ include file is in.

Traditional make:

You can download the Eigen3 library manually if you prefer; follow the instructions in lib/smd/README. You can also do it in one step from the lammps/src dir, using a command like these, which simply invoke the lib/smd/Install.py script with the specified args:

```
$ make lib-smd                          # print help message
$ make lib-smd args="-b"                # download to lib/smd/eigen3
$ make lib-smd args="-p /usr/include/eigen3"    # use existing Eigen installation in /
↪usr/include/eigen3
```

Note that a symbolic (soft) link named "includelink" is created in lib/smd to point to the Eigen dir. When LAMMPS builds it will use this link. You should not need to edit the lib/smd/Makefile.lammps file.

3.7.26 USER-VTK package

To build with this package you must have the VTK library installed on your system.

CMake build:

No additional settings are needed besides "-D PKG_USER-VTK=yes".

This should auto-detect the VTK library if it is installed on your system at standard locations. Several advanced VTK options exist if you need to specify where it was installed. Use the ccmake (terminal window) or cmake-gui (graphical) tools to see these options and set them interactively from their user interfaces.

Traditional make:

The lib/vtk/Makefile.lammps file has settings for accessing VTK files and its library, which LAMMPS needs to build with this package. If the settings are not valid for your system, check if one of the other lib/vtk/Makefile.lammps.* files is compatible and copy it to Makefile.lammps. If none of the provided files work, you will need to edit the Makefile.lammps file. See lib/vtk/README for details.

3.8 Notes for building LAMMPS on Windows

- *General remarks*
- *Running Linux on Windows*
- *Using GNU GCC ported to Windows*
- *Using a cross-compiler*

3.8.1 General remarks

LAMMPS is developed and tested primarily on Linux machines. The vast majority of HPC clusters and supercomputers today runs on Linux as well. While portability to other platforms is desired, it is not always achieved. The LAMMPS developers strongly rely on LAMMPS users giving feedback and providing assistance in resolving portability issues. This is particularly true for compiling LAMMPS on Windows, since this platform has significant differences with some low-level functionality.

3.8.2 Running Linux on Windows

So before trying to build LAMMPS on Windows, please consider if using the pre-compiled Windows binary packages are sufficient for your needs (as an aside, those packages themselves are build on a Linux machine using cross-compilers). If it is necessary for you to compile LAMMPS on a Windows machine (e.g. because it is your main desktop), please also consider using a virtual machine software and compile and run LAMMPS in a Linux virtual machine, or - if you have a recently updated Windows 10 installation - consider using the Windows subsystem for Linux. This optional Windows feature allows you to run the bash shell from Ubuntu from within Windows and from there on, you can pretty much use that shell like you are running on an Ubuntu Linux machine (e.g. installing software via apt-get and more). For more details on that, please see *this tutorial*

3.8.3 Using a GNU GCC ported to Windows

One option for compiling LAMMPS on Windows natively, that has been known to work in the past is to install a bash shell, unix shell utilities, perl, GNU make, and a GNU compiler ported to Windows. The Cygwin package provides a unix/linux interface to low-level Windows functions, so LAMMPS can be compiled on Windows. The necessary (minor) modifications to LAMMPS are included, but may not always up-to-date for recently added functionality and the corresponding new code. A machine makefile for using cygwin for the old build system is provided. Using CMake for this mode of compilation is untested and not likely to work.

When compiling for Windows do **not** set the -DLAMMPS_MEMALIGN define in the LMP_INC makefile variable and add -lwsock32 -lpsapi to the linker flags in LIB makefile variable. Try adding -static-libgcc or -static or both to the linker flags when your resulting LAMMPS Windows executable complains about missing .dll files. The CMake configuration should set this up automatically, but is untested.

In case of problems, you are recommended to contact somebody with experience in using cygwin. If you do come across portability problems requiring changes to the LAMMPS source code, or figure out corrections yourself, please report them on the lammps-users mailing list, or file them as an issue or pull request on the LAMMPS GitHub project.

3.8.4 Using a cross-compiler

If you need to provide custom LAMMPS binaries for Windows, but do not need to do the compilation on Windows, please consider using a Linux to Windows cross-compiler. This is how currently the Windows binary packages are created by the LAMMPS developers. Because of that, this is probably the currently best tested and supported way to build LAMMPS executables for Windows. There are makefiles provided for the traditional build system, but CMake has also been successfully tested using the mingw32-cmake and mingw64-cmake wrappers that are bundled with the cross-compiler environment on Fedora machines. A CMake preset selecting all packages compatible with this cross-compilation build is provided. You will likely need to disable the GPU package unless you download and install the contents of the pre-compiled OpenCL ICD loader library into your MinGW64 cross-compiler environment. The cross-compilation currently will only produce non-MPI serial binaries.

Please keep in mind, though, that this only applies to **compiling** LAMMPS. Whether the resulting binaries do work correctly is not tested by the LAMMPS developers. We instead rely on the feedback of the users of these pre-compiled LAMMPS packages for Windows. We will try to resolve issues to the best of our abilities if we become aware of them. However this is subject to time constraints and focus on HPC platforms.

3.8.5 Native Visual C++ support

Support for the Visual C++ compilers is currently not available. The CMake build system is capable of creating suitable a Visual Studio style build environment, but the LAMMPS code itself is not fully ported to support Visual C++. Volunteers to take on this task are welcome.

3.9 Development build options (CMake only)

The CMake build of LAMMPS has a few extra options which are useful during development, testing or debugging.

3.9.1 Verify compilation flags

Sometimes it is necessary to verify the complete sequence of compilation flags generated by the CMake build. To enable a more verbose output during compilation you can use the following option.

```
-D CMAKE_VERBOSE_MAKEFILE=value     # value = no (default) or yes
```

Another way of doing this without reconfiguration is calling make with variable VERBOSE set to 1:

```
make VERBOSE=1
```

3.9.2 Address, Undefined Behavior, and Thread Sanitizer Support

Compilers such as GCC and Clang support generating binaries which use different sanitizers to detect problems in code during run-time. They can detect memory leaks, code that runs into undefined behavior of the language and data races in threaded code.

The following settings allow you enable these features if your compiler supports it. Please note that they come with a performance hit. However, they are usually faster than using tools like Valgrind.

```
-D ENABLE_SANITIZE_ADDRESS=value     # enable Address Sanitizer, value = no (default)␣
↪or yes
-D ENABLE_SANITIZE_UNDEFINED=value   # enable Undefined Behaviour Sanitizer, value =␣
↪no (default) or yes
-D ENABLE_SANITIZE_THREAD=value      # enable Thread Sanitizer, value = no (default)␣
↪or yes
```

3.9.3 Code Coverage and Testing

We do extensive regression testing of the LAMMPS code base on a continuous basis. Some of the logic to do this has been added to the CMake build so developers can run the tests directly on their workstation.

Note: this is incomplete and only represents a small subset of tests that we run

```
-D ENABLE_TESTING=value                # enable simple run tests of LAMMPS, value = no␣
↪(default) or yes
-D LAMMPS_TESTING_SOURCE_DIR=path      # path to lammps-testing repository (option if␣
↪in custom location)
-D LAMMPS_TESTING_GIT_TAG=value        # version of lammps-testing repository that␣
↪should be used, value = master (default) or custom git commit or tag
```

If you enable testing in the CMake build it will create an additional target called "test". You can run them with:

```
make test
```

The test cases used come from the lammps-testing repository. They are derivatives of the examples folder with some modifications to make the run faster.

You can also collect code coverage metrics while running the tests by enabling coverage support during building.

```
-D ENABLE_COVERAGE=value  # enable coverage measurements, value = no (default) or yes
```

This will also add the following targets to generate coverage reports after running the LAMMPS executable:

```
make test                # run tests first!
make gen_coverage_html   # generate coverage report in HTML format
make gen_coverage_xml    # generate coverage report in XML format
```

These reports require GCOVR to be installed. The easiest way to do this to install it via pip:

```
pip install git+https://github.com/gcovr/gcovr.git
```

CHAPTER

FOUR

RUN LAMMPS

These pages explain how to run LAMMPS once you have *installed an executable* or *downloaded the source code* and *built an executable*. The *Commands* doc page describes how input scripts are structured and the commands they can contain.

4.1 Basics of running LAMMPS

LAMMPS is run from the command line, reading commands from a file via the -in command line flag, or from standard input. Using the "-in in.file" variant is recommended:

```
$ lmp_serial -in in.file
$ lmp_serial < in.file
$ /path/to/lammps/src/lmp_serial -i in.file
$ mpirun -np 4 lmp_mpi -in in.file
$ mpirun -np 8 /path/to//lammps/src/lmp_mpi -in in.file
$ mpirun -np 6 /usr/local/bin/lmp -in in.file
```

You normally run the LAMMPS command in the directory where your input script is located. That is also where output files are produced by default, unless you provide specific other paths in your input script or on the command line. As in some of the examples above, the LAMMPS executable itself can be placed elsewhere.

Note: The redirection operator "<" will not always work when running in parallel with mpirun; for those systems the -in form is required.

As LAMMPS runs it prints info to the screen and a logfile named *log.lammps*. More info about output is given on the *Run output* doc page.

If LAMMPS encounters errors in the input script or while running a simulation it will print an ERROR message and stop or a WARNING message and continue. See the *Errors* doc page for a discussion of the various kinds of errors LAMMPS can or can't detect, a list of all ERROR and WARNING messages, and what to do about them.

LAMMPS can run the same problem on any number of processors, including a single processor. In theory you should get identical answers on any number of processors and on any machine. In practice, numerical round-off due to using floating-point math can cause slight differences and an eventual divergence of molecular dynamics trajectories. See the *Errors common* doc page for discussion of this.

LAMMPS can run as large a problem as will fit in the physical memory of one or more processors. If you run out of memory, you must run on more processors or define a smaller problem. The amount of memory needed and how well it can be distributed across processors may vary based on the models and settings and commands used.

If you run LAMMPS in parallel via mpirun, you should be aware of the *processors* command, which controls how MPI tasks are mapped to the simulation box, as well as mpirun options that control how MPI tasks are assigned to physical cores of the node(s) of the machine you are running on. These settings can improve performance, though the defaults are often adequate.

For example, it is often important to bind MPI tasks (processes) to physical cores (processor affinity), so that the operating system does not migrate them during a simulation. If this is not the default behavior on your machine, the mpirun option "–bind-to core" (OpenMPI) or "-bind-to core" (MPICH) can be used.

If the LAMMPS command(s) you are using support multi-threading, you can set the number of threads per MPI task via the environment variable OMP_NUM_THREADS, before you launch LAMMPS:

```
$ export OMP_NUM_THREADS=2      # bash
$ setenv OMP_NUM_THREADS 2      # csh or tcsh
```

This can also be done via the *package* command or via the *-pk command-line switch* which invokes the package command. See the *package* command or *Speed* doc pages for more details about which accelerator packages and which commands support multi-threading.

You can experiment with running LAMMPS using any of the input scripts provided in the examples or bench directory. Input scripts are named in.* and sample outputs are named log.*.P where P is the number of processors it was run on.

Some of the examples or benchmarks require LAMMPS to be built with optional packages.

4.2 Command-line options

At run time, LAMMPS recognizes several optional command-line switches which may be used in any order. Either the full word or a one-or-two letter abbreviation can be used:

- *-e or -echo*
- *-h or -help*
- *-i or -in*
- *-k or -kokkos*
- *-l or -log*
- *-m or -mpicolor*
- *-nc or -nocite*
- *-pk or -package*
- *-p or -partition*
- *-pl or -plog*
- *-ps or -pscreen*
- *-ro or -reorder*
- *-r2data or -restart2data*
- *-r2dump or -restart2dump*
- *-sc or -screen*
- *-sf or -suffix*
- *-v or -var*

For example, the lmp_mpi executable might be launched as follows:

```
$ mpirun -np 16 lmp_mpi -v f tmp.out -l my.log -sc none -i in.alloy
$ mpirun -np 16 lmp_mpi -var f tmp.out -log my.log -screen none -in in.alloy
```

-echo style

Set the style of command echoing. The style can be *none* or *screen* or *log* or *both*. Depending on the style, each command read from the input script will be echoed to the screen and/or logfile. This can be useful to figure out which line of your script is causing an input error. The default value is *log*. The echo style can also be set by using the *echo* command in the input script itself.

-help

Print a brief help summary and a list of options compiled into this executable for each LAMMPS style (atom_style, fix, compute, pair_style, bond_style, etc). This can tell you if the command you want to use was included via the appropriate package at compile time. LAMMPS will print the info and immediately exit if this switch is used.

-in file

Specify a file to use as an input script. This is an optional switch when running LAMMPS in one-partition mode. If it is not specified, LAMMPS reads its script from standard input, typically from a script via I/O redirection; e.g. lmp_linux < in.run. I/O redirection should also work in parallel, but if it does not (in the unlikely case that an MPI implementation does not support it), then use the -in flag. Note that this is a required switch when running LAMMPS in multi-partition mode, since multiple processors cannot all read from stdin.

-kokkos on/off keyword/value ...

Explicitly enable or disable KOKKOS support, as provided by the KOKKOS package. Even if LAMMPS is built with this package, as described in *Speed kokkos*, this switch must be set to enable running with KOKKOS-enabled styles the package provides. If the switch is not set (the default), LAMMPS will operate as if the KOKKOS package were not installed; i.e. you can run standard LAMMPS or with the GPU or USER-OMP packages, for testing or benchmarking purposes.

Additional optional keyword/value pairs can be specified which determine how Kokkos will use the underlying hardware on your platform. These settings apply to each MPI task you launch via the "mpirun" or "mpiexec" command. You may choose to run one or more MPI tasks per physical node. Note that if you are running on a desktop machine, you typically have one physical node. On a cluster or supercomputer there may be dozens or 1000s of physical nodes.

Either the full word or an abbreviation can be used for the keywords. Note that the keywords do not use a leading minus sign. I.e. the keyword is "t", not "-t". Also note that each of the keywords has a default setting. Examples of when to use these options and what settings to use on different platforms is given on the *Speed kokkos* doc page.

- d or device
- g or gpus
- t or threads
- n or numa

```
device Nd
```

This option is only relevant if you built LAMMPS with CUDA=yes, you have more than one GPU per node, and if you are running with only one MPI task per node. The Nd setting is the ID of the GPU on the node to run on. By default Nd = 0. If you have multiple GPUs per node, they have consecutive IDs numbered as 0,1,2,etc. This setting allows you to launch multiple independent jobs on the node, each with a single MPI task per node, and assign each job to run on a different GPU.

```
gpus Ng Ns
```

This option is only relevant if you built LAMMPS with CUDA=yes, you have more than one GPU per node, and you are running with multiple MPI tasks per node (up to one per GPU). The Ng setting is how many GPUs you will use. The Ns setting is optional. If set, it is the ID of a GPU to skip when assigning MPI tasks to GPUs. This may be useful if your desktop system reserves one GPU to drive the screen and the rest are intended for computational work like running LAMMPS. By default Ng = 1 and Ns is not set.

Depending on which flavor of MPI you are running, LAMMPS will look for one of these 4 environment variables

```
SLURM_LOCALID (various MPI variants compiled with SLURM support)
MPT_LRANK (HPE MPI)
MV2_COMM_WORLD_LOCAL_RANK (Mvapich)
OMPI_COMM_WORLD_LOCAL_RANK (OpenMPI)
```

which are initialized by the "srun", "mpirun" or "mpiexec" commands. The environment variable setting for each MPI rank is used to assign a unique GPU ID to the MPI task.

```
threads Nt
```

This option assigns Nt number of threads to each MPI task for performing work when Kokkos is executing in OpenMP or pthreads mode. The default is Nt = 1, which essentially runs in MPI-only mode. If there are Np MPI tasks per physical node, you generally want Np*Nt = the number of physical cores per node, to use your available hardware optimally. This also sets the number of threads used by the host when LAMMPS is compiled with CUDA=yes.

```
numa Nm
```

This option is only relevant when using pthreads with hwloc support. In this case Nm defines the number of NUMA regions (typically sockets) on a node which will be utilized by a single MPI rank. By default Nm = 1. If this option is used the total number of worker-threads per MPI rank is threads*numa. Currently it is always almost better to assign at least one MPI rank per NUMA region, and leave numa set to its default value of 1. This is because letting a single process span multiple NUMA regions induces a significant amount of cross NUMA data traffic which is slow.

-log file

Specify a log file for LAMMPS to write status information to. In one-partition mode, if the switch is not used, LAMMPS writes to the file log.lammps. If this switch is used, LAMMPS writes to the specified file. In multi-partition mode, if the switch is not used, a log.lammps file is created with high-level status information. Each partition also writes to a log.lammps.N file where N is the partition ID. If the switch is specified in multi-partition mode, the high-level logfile is named "file" and each partition also logs information to a file.N. For both one-partition and multi-partition mode, if the specified file is "none", then no log files are created. Using a *log* command in the input script will override this setting. Option -plog will override the name of the partition log files file.N.

-mpicolor color

If used, this must be the first command-line argument after the LAMMPS executable name. It is only used when LAMMPS is launched by an mpirun command which also launches another executable(s) at the same time. (The other executable could be LAMMPS as well.) The color is an integer value which should be different for each executable (another application may set this value in a different way). LAMMPS and the other executable(s) perform

an MPI_Comm_split() with their own colors to shrink the MPI_COMM_WORLD communication to be the subset of processors they are actually running on.

Currently, this is only used in LAMMPS to perform client/server messaging with another application. LAMMPS can act as either a client or server (or both). More details are given on the *Howto client/server* doc page.

Specifically, this refers to the "mpi/one" mode of messaging provided by the *message* command and the CSlib library LAMMPS links with from the lib/message directory. See the *message* command for more details.

-nocite

Disable writing the log.cite file which is normally written to list references for specific cite-able features used during a LAMMPS run. See the citation page for more details.

-package style args . . . .

Invoke the *package* command with style and args. The syntax is the same as if the command appeared at the top of the input script. For example "-package gpu 2" or "-pk gpu 2" is the same as *package gpu 2* in the input script. The possible styles and args are documented on the *package* doc page. This switch can be used multiple times, e.g. to set options for the USER-INTEL and USER-OMP packages which can be used together.

Along with the "-suffix" command-line switch, this is a convenient mechanism for invoking accelerator packages and their options without having to edit an input script.

-partition 8x2 4 5 . . .

Invoke LAMMPS in multi-partition mode. When LAMMPS is run on P processors and this switch is not used, LAMMPS runs in one partition, i.e. all P processors run a single simulation. If this switch is used, the P processors are split into separate partitions and each partition runs its own simulation. The arguments to the switch specify the number of processors in each partition. Arguments of the form MxN mean M partitions, each with N processors. Arguments of the form N mean a single partition with N processors. The sum of processors in all partitions must equal P. Thus the command "-partition 8x2 4 5" has 10 partitions and runs on a total of 25 processors.

Running with multiple partitions can be useful for running *multi-replica simulations*, where each replica runs on one or a few processors. Note that with MPI installed on a machine (e.g. your desktop), you can run on more (virtual) processors than you have physical processors.

To run multiple independent simulations from one input script, using multiple partitions, see the *Howto multiple* doc page. World- and universe-style *variables* are useful in this context.

-plog file

Specify the base name for the partition log files, so partition N writes log information to file.N. If file is none, then no partition log files are created. This overrides the filename specified in the -log command-line option. This option is useful when working with large numbers of partitions, allowing the partition log files to be suppressed (-plog none) or placed in a sub-directory (-plog replica_files/log.lammps) If this option is not used the log file for partition N is log.lammps.N or whatever is specified by the -log command-line option.

-pscreen file

Specify the base name for the partition screen file, so partition N writes screen information to file.N. If file is none, then no partition screen files are created. This overrides the filename specified in the -screen command-line option. This option is useful when working with large numbers of partitions, allowing the partition screen files to be suppressed

(-pscreen none) or placed in a sub-directory (-pscreen replica_files/screen). If this option is not used the screen file for partition N is screen.N or whatever is specified by the -screen command-line option.

-reorder

This option has 2 forms:

```
-reorder nth N
-reorder custom filename
```

Reorder the processors in the MPI communicator used to instantiate LAMMPS, in one of several ways. The original MPI communicator ranks all P processors from 0 to P-1. The mapping of these ranks to physical processors is done by MPI before LAMMPS begins. It may be useful in some cases to alter the rank order. E.g. to insure that cores within each node are ranked in a desired order. Or when using the *run_style verlet/split* command with 2 partitions to insure that a specific Kspace processor (in the 2nd partition) is matched up with a specific set of processors in the 1st partition. See the *Speed tips* doc page for more details.

If the keyword *nth* is used with a setting *N*, then it means every Nth processor will be moved to the end of the ranking. This is useful when using the *run_style verlet/split* command with 2 partitions via the -partition command-line switch. The first set of processors will be in the first partition, the 2nd set in the 2nd partition. The -reorder command-line switch can alter this so that the 1st N procs in the 1st partition and one proc in the 2nd partition will be ordered consecutively, e.g. as the cores on one physical node. This can boost performance. For example, if you use "-reorder nth 4" and "-partition 9 3" and you are running on 12 processors, the processors will be reordered from

```
0 1 2 3 4 5 6 7 8 9 10 11
```

to

```
0 1 2 4 5 6 8 9 10 3 7 11
```

so that the processors in each partition will be

```
0 1 2 4 5 6 8 9 10
3 7 11
```

See the "processors" command for how to insure processors from each partition could then be grouped optimally for quad-core nodes.

If the keyword is *custom*, then a file that specifies a permutation of the processor ranks is also specified. The format of the reorder file is as follows. Any number of initial blank or comment lines (starting with a "#" character) can be present. These should be followed by P lines of the form:

```
I J
```

where P is the number of processors LAMMPS was launched with. Note that if running in multi-partition mode (see the -partition switch above) P is the total number of processors in all partitions. The I and J values describe a permutation of the P processors. Every I and J should be values from 0 to P-1 inclusive. In the set of P I values, every proc ID should appear exactly once. Ditto for the set of P J values. A single I,J pairing means that the physical processor with rank I in the original MPI communicator will have rank J in the reordered communicator.

Note that rank ordering can also be specified by many MPI implementations, either by environment variables that specify how to order physical processors, or by config files that specify what physical processors to assign to each MPI rank. The -reorder switch simply gives you a portable way to do this without relying on MPI itself. See the *processors out* command for how to output info on the final assignment of physical processors to the LAMMPS simulation domain.

-restart2data restartfile [remap] datafile keyword value ...

Convert the restart file into a data file and immediately exit. This is the same operation as if the following 2-line input script were run:

```
read_restart restartfile [remap]
write_data datafile keyword value ...
```

The specified restartfile and/or datafile name may contain the wild-card character "*". The restartfile name may also contain the wild-card character "%". The meaning of these characters is explained on the *read_restart* and *write_data* doc pages. The use of "%" means that a parallel restart file can be read. Note that a filename such as file.* may need to be enclosed in quotes or the "*" character prefixed with a backslash ("") to avoid shell expansion of the "*" character.

Following restartfile argument, the optional word "remap" may be used. This has the same effect like adding it to a *read_restart* command, and operates as explained on its doc page. This is useful if reading the restart file triggers an error that atoms have been lost. In that case, use of the remap flag should allow the data file to still be produced.

The syntax following restartfile (or remap), namely

```
datafile keyword value ...
```

is identical to the arguments of the *write_data* command. See its doc page for details. This includes its optional keyword/value settings.

-restart2dump restartfile [remap] group-ID dumpstyle dumpfile arg1 arg2 ...

Convert the restart file into a dump file and immediately exit. This is the same operation as if the following 2-line input script were run:

```
read_restart restartfile [remap]
write_dump group-ID dumpstyle dumpfile arg1 arg2 ...
```

Note that the specified restartfile and dumpfile names may contain wild-card characters ("*","%") as explained on the *read_restart* and *write_dump* doc pages. The use of "%" means that a parallel restart file and/or parallel dump file can be read and/or written. Note that a filename such as file.* may need to be enclosed in quotes or the "*" character prefixed with a backslash ("") to avoid shell expansion of the "*" character.

Note that following the restartfile argument, the optional word "remap" can be used. This has the effect as adding it to the *read_restart* command, as explained on its doc page. This is useful if reading the restart file triggers an error that atoms have been lost. In that case, use of the remap flag should allow the dump file to still be produced.

The syntax following restartfile (or remap), namely

```
group-ID dumpstyle dumpfile arg1 arg2 ...
```

is identical to the arguments of the *write_dump* command. See its doc page for details. This includes what per-atom fields are written to the dump file and optional dump_modify settings, including ones that affect how parallel dump files are written, e.g. the *nfile* and *fileper* keywords. See the *dump_modify* doc page for details.

-screen file

Specify a file for LAMMPS to write its screen information to. In one-partition mode, if the switch is not used, LAMMPS writes to the screen. If this switch is used, LAMMPS writes to the specified file instead and you will see no screen output. In multi-partition mode, if the switch is not used, high-level status information is written to the screen. Each partition also writes to a screen.N file where N is the partition ID. If the switch is specified in multi-partition mode, the high-level screen dump is named "file" and each partition also writes screen information to a file.N. For

both one-partition and multi-partition mode, if the specified file is "none", then no screen output is performed. Option -pscreen will override the name of the partition screen files file.N.

-suffix style args

Use variants of various styles if they exist. The specified style can be *gpu*, *intel*, *kk*, *omp*, *opt*, or *hybrid*. These refer to optional packages that LAMMPS can be built with, as described in *Accelerate performance*. The "gpu" style corresponds to the GPU package, the "intel" style to the USER-INTEL package, the "kk" style to the KOKKOS package, the "opt" style to the OPT package, and the "omp" style to the USER-OMP package. The hybrid style is the only style that accepts arguments. It allows for two packages to be specified. The first package specified is the default and will be used if it is available. If no style is available for the first package, the style for the second package will be used if available. For example, "-suffix hybrid intel omp" will use styles from the USER-INTEL package if they are installed and available, but styles for the USER-OMP package otherwise.

Along with the "-package" command-line switch, this is a convenient mechanism for invoking accelerator packages and their options without having to edit an input script.

As an example, all of the packages provide a *pair_style lj/cut* variant, with style names lj/cut/gpu, lj/cut/intel, lj/cut/kk, lj/cut/omp, and lj/cut/opt. A variant style can be specified explicitly in your input script, e.g. pair_style lj/cut/gpu. If the -suffix switch is used the specified suffix (gpu,intel,kk,omp,opt) is automatically appended whenever your input script command creates a new *atom*, *pair*, *fix*, *compute*, or *run* style. If the variant version does not exist, the standard version is created.

For the GPU package, using this command-line switch also invokes the default GPU settings, as if the command "package gpu 1" were used at the top of your input script. These settings can be changed by using the "-package gpu" command-line switch or the *package gpu* command in your script.

For the USER-INTEL package, using this command-line switch also invokes the default USER-INTEL settings, as if the command "package intel 1" were used at the top of your input script. These settings can be changed by using the "-package intel" command-line switch or the *package intel* command in your script. If the USER-OMP package is also installed, the hybrid style with "intel omp" arguments can be used to make the omp suffix a second choice, if a requested style is not available in the USER-INTEL package. It will also invoke the default USER-OMP settings, as if the command "package omp 0" were used at the top of your input script. These settings can be changed by using the "-package omp" command-line switch or the *package omp* command in your script.

For the KOKKOS package, using this command-line switch also invokes the default KOKKOS settings, as if the command "package kokkos" were used at the top of your input script. These settings can be changed by using the "-package kokkos" command-line switch or the *package kokkos* command in your script.

For the OMP package, using this command-line switch also invokes the default OMP settings, as if the command "package omp 0" were used at the top of your input script. These settings can be changed by using the "-package omp" command-line switch or the *package omp* command in your script.

The *suffix* command can also be used within an input script to set a suffix, or to turn off or back on any suffix setting made via the command line.

-var name value1 value2 . . .

Specify a variable that will be defined for substitution purposes when the input script is read. This switch can be used multiple times to define multiple variables. "Name" is the variable name which can be a single character (referenced as $x in the input script) or a full string (referenced as ${abc}). An *index-style variable* will be created and populated with the subsequent values, e.g. a set of filenames. Using this command-line option is equivalent to putting the line "variable name index value1 value2 . . ." at the beginning of the input script. Defining an index variable as a command-line argument overrides any setting for the same index variable in the input script, since index variables cannot be re-defined.

See the *variable* command for more info on defining index and other kinds of variables and the *Commands parse* page for more info on using variables in input scripts.

Note: Currently, the command-line parser looks for arguments that start with "-" to indicate new switches. Thus you cannot specify multiple variable values if any of them start with a "-", e.g. a negative numeric value. It is OK if the first value1 starts with a "-", since it is automatically skipped.

4.3 Screen and logfile output

As LAMMPS reads an input script, it prints information to both the screen and a log file about significant actions it takes to setup a simulation. When the simulation is ready to begin, LAMMPS performs various initializations, and prints info about the run it is about to perform, including the amount of memory (in MBytes per processor) that the simulation requires. It also prints details of the initial thermodynamic state of the system. During the run itself, thermodynamic information is printed periodically, every few timesteps. When the run concludes, LAMMPS prints the final thermodynamic state and a total run time for the simulation. It also appends statistics about the CPU time and storage requirements for the simulation. An example set of statistics is shown here:

```
Loop time of 2.81192 on 4 procs for 300 steps with 2004 atoms

Performance: 18.436 ns/day  1.302 hours/ns  106.689 timesteps/s
97.0% CPU use with 4 MPI tasks x no OpenMP threads

MPI task timings breakdown:
Section |  min time  |  avg time  |  max time  |%varavg| %total
---------------------------------------------------------------
Pair    | 1.9808     | 2.0134     | 2.0318     |   1.4 | 71.60
Bond    | 0.0021894  | 0.0060319  | 0.010058   |   4.7 |  0.21
Kspace  | 0.3207     | 0.3366     | 0.36616    |   3.1 | 11.97
Neigh   | 0.28411    | 0.28464    | 0.28516    |   0.1 | 10.12
Comm    | 0.075732   | 0.077018   | 0.07883    |   0.4 |  2.74
Output  | 0.00030518 | 0.00042665 | 0.00078821 |   1.0 |  0.02
Modify  | 0.086606   | 0.086631   | 0.086668   |   0.0 |  3.08
Other   |            | 0.007178   |            |       |  0.26

Nlocal:    501 ave 508 max 490 min
Histogram: 1 0 0 0 0 0 1 1 0 1
Nghost:    6586.25 ave 6628 max 6548 min
Histogram: 1 0 1 0 0 0 1 0 0 1
Neighs:    177007 ave 180562 max 170212 min
Histogram: 1 0 0 0 0 0 0 1 1 1

Total # of neighbors = 708028
Ave neighs/atom = 353.307
Ave special neighs/atom = 2.34032
Neighbor list builds = 26
Dangerous builds = 0
```

The first section provides a global loop timing summary. The *loop time* is the total wall-clock time for the simulation to run. The *Performance* line is provided for convenience to help predict how long it will take to run a desired physical simulation. The *CPU use* line provides the CPU utilization per MPI task; it should be close to 100% times the number

of OpenMP threads (or 1 of not using OpenMP). Lower numbers correspond to delays due to file I/O or insufficient thread utilization.

The *MPI task* section gives the breakdown of the CPU run time (in seconds) into major categories:

- *Pair* = non-bonded force computations
- *Bond* = bonded interactions: bonds, angles, dihedrals, impropers
- *Kspace* = long-range interactions: Ewald, PPPM, MSM
- *Neigh* = neighbor list construction
- *Comm* = inter-processor communication of atoms and their properties
- *Output* = output of thermodynamic info and dump files
- *Modify* = fixes and computes invoked by fixes
- *Other* = all the remaining time

For each category, there is a breakdown of the least, average and most amount of wall time any processor spent on this category of computation. The "%varavg" is the percentage by which the max or min varies from the average. This is an indication of load imbalance. A percentage close to 0 is perfect load balance. A large percentage is imbalance. The final "%total" column is the percentage of the total loop time is spent in this category.

When using the *timer full* setting, an additional column is added that also prints the CPU utilization in percent. In addition, when using *timer full* and the *package omp* command are active, a similar timing summary of time spent in threaded regions to monitor thread utilization and load balance is provided. A new *Thread timings* section is also added, which lists the time spent in reducing the per-thread data elements to the storage for non-threaded computation. These thread timings are measured for the first MPI rank only and thus, because the breakdown for MPI tasks can change from MPI rank to MPI rank, this breakdown can be very different for individual ranks. Here is an example output for this section:

```
Thread timings breakdown (MPI rank 0):
Total threaded time 0.6846 / 90.6%
Section |  min time  |  avg time  |  max time  |%varavg| %total
--------------------------------------------------------------
Pair    | 0.5127     | 0.5147     | 0.5167     |   0.3 | 75.18
Bond    | 0.0043139  | 0.0046779  | 0.0050418  |   0.5 |  0.68
Kspace  | 0.070572   | 0.074541   | 0.07851    |   1.5 | 10.89
Neigh   | 0.084778   | 0.086969   | 0.089161   |   0.7 | 12.70
Reduce  | 0.0036485  | 0.003737   | 0.0038254  |   0.1 |  0.55
```

The third section above lists the number of owned atoms (Nlocal), ghost atoms (Nghost), and pair-wise neighbors stored per processor. The max and min values give the spread of these values across processors with a 10-bin histogram showing the distribution. The total number of histogram counts is equal to the number of processors.

The last section gives aggregate statistics (across all processors) for pair-wise neighbors and special neighbors that LAMMPS keeps track of (see the *special_bonds* command). The number of times neighbor lists were rebuilt is tallied, as is the number of potentially *dangerous* rebuilds. If atom movement triggered neighbor list rebuilding (see the *neigh_modify* command), then dangerous reneighborings are those that were triggered on the first timestep atom movement was checked for. If this count is non-zero you may wish to reduce the delay factor to insure no force interactions are missed by atoms moving beyond the neighbor skin distance before a rebuild takes place.

If an energy minimization was performed via the *minimize* command, additional information is printed, e.g.

```
Minimization stats:
  Stopping criterion = linesearch alpha is zero
  Energy initial, next-to-last, final =
        -6372.3765206     -8328.46998942     -8328.46998942
  Force two-norm initial, final = 1059.36 5.36874
  Force max component initial, final = 58.6026 1.46872
  Final line search alpha, max atom move = 2.7842e-10 4.0892e-10
  Iterations, force evaluations = 701 1516
```

The first line prints the criterion that determined minimization was converged. The next line lists the initial and final energy, as well as the energy on the next-to-last iteration. The next 2 lines give a measure of the gradient of the energy (force on all atoms). The 2-norm is the "length" of this 3N-component force vector; the largest component (x, y, or z) of force (infinity-norm) is also given. Then information is provided about the line search and statistics on how many iterations and force-evaluations the minimizer required. Multiple force evaluations are typically done at each iteration to perform a 1d line minimization in the search direction. See the *minimize* doc page for more details.

If a *kspace_style* long-range Coulombics solver that performs FFTs was used during the run (PPPM, Ewald), then additional information is printed, e.g.

```
FFT time (% of Kspce) = 0.200313 (8.34477)
FFT Gflps 3d 1d-only = 2.31074 9.19989
```

The first line is the time spent doing 3d FFTs (several per timestep) and the fraction it represents of the total KSpace time (listed above). Each 3d FFT requires computation (3 sets of 1d FFTs) and communication (transposes). The total flops performed is 5Nlog_2(N), where N is the number of points in the 3d grid. The FFTs are timed with and without the communication and a Gflop rate is computed. The 3d rate is with communication; the 1d rate is without (just the 1d FFTs). Thus you can estimate what fraction of your FFT time was spent in communication, roughly 75% in the example above.

4.4 Running LAMMPS on Windows

To run a serial (non-MPI) executable, follow these steps:

- Get a command prompt by going to Start->Run... , then typing "cmd".
- Move to the directory where you have your input script, (e.g. by typing: cd "Documents").
- At the command prompt, type "lmp_serial -in in.file", where in.file is the name of your LAMMPS input script.

Note that the serial executable includes support for multi-threading parallelization from the styles in the USER-OMP packages. To run with 4 threads, you can type this:

```
lmp_serial -in in.lj -pk omp 4 -sf omp
```

For the MPI executable, which allows you to run LAMMPS under Windows in parallel, follow these steps.

Download and install a compatible MPI library binary package:

- for 32-bit Windows: mpich2-1.4.1p1-win-ia32.msi
- for 64-bit Windows: mpich2-1.4.1p1-win-x86-64.msi

The LAMMPS Windows installer packages will automatically adjust your path for the default location of this MPI package. After the installation of the MPICH2 software, it needs to be integrated into the system. For this you need to start a Command Prompt in *Administrator Mode* (right click on the icon and select it). Change into the MPICH2 installation directory, then into the sub-directory **bin** and execute **smpd.exe -install**. Exit the command window.

- Get a new, regular command prompt by going to Start->Run... , then typing "cmd".
- Move to the directory where you have your input file (e.g. by typing: cd "Documents").

Then type something like this:

```
mpiexec -localonly 4 lmp_mpi -in in.file
mpiexec -np 4 lmp_mpi -in in.file
```

where in.file is the name of your LAMMPS input script. For the latter case, you may be prompted to enter your password.

In this mode, output may not immediately show up on the screen, so if your input script takes a long time to execute, you may need to be patient before the output shows up.

The parallel executable can also run on a single processor by typing something like this:

```
lmp_mpi -in in.lj
```

Note that the parallel executable also includes OpenMP multi-threading, which can be combined with MPI using something like:

```
mpiexec -localonly 2 lmp_mpi -in in.lj -pk omp 2 -sf omp
```

CHAPTER

FIVE

COMMANDS

These pages describe how a LAMMPS input script is formatted and the commands in it are used to define a LAMMPS simulation.

5.1 LAMMPS input scripts

LAMMPS executes by reading commands from a input script (text file), one line at a time. When the input script ends, LAMMPS exits. Each command causes LAMMPS to take some action. It may set an internal variable, read in a file, or run a simulation. Most commands have default settings, which means you only need to use the command if you wish to change the default.

In many cases, the ordering of commands in an input script is not important. However the following rules apply:

(1) LAMMPS does not read your entire input script and then perform a simulation with all the settings. Rather, the input script is read one line at a time and each command takes effect when it is read. Thus this sequence of commands:

```
timestep 0.5
run      100
run      100
```

does something different than this sequence:

```
run      100
timestep 0.5
run      100
```

In the first case, the specified timestep (0.5 fs) is used for two simulations of 100 timesteps each. In the 2nd case, the default timestep (1.0 fs) is used for the 1st 100 step simulation and a 0.5 fs timestep is used for the 2nd one.

(2) Some commands are only valid when they follow other commands. For example you cannot set the temperature of a group of atoms until atoms have been defined and a group command is used to define which atoms belong to the group.

(3) Sometimes command B will use values that can be set by command A. This means command A must precede command B in the input script if it is to have the desired effect. For example, the *read_data* command initializes the system by setting up the simulation box and assigning atoms to processors. If default values are not desired, the *processors* and *boundary* commands need to be used before read_data to tell LAMMPS how to map processors to the simulation box.

Many input script errors are detected by LAMMPS and an ERROR or WARNING message is printed. The *Errors* doc page gives more information on what errors mean. The documentation for each command lists restrictions on how the command can be used.

5.2 Parsing rules for input scripts

Each non-blank line in the input script is treated as a command. LAMMPS commands are case sensitive. Command names are lower-case, as are specified command arguments. Upper case letters may be used in file names or user-chosen ID strings.

Here are 6 rules for how each line in the input script is parsed by LAMMPS:

1. If the last printable character on the line is a "&" character, the command is assumed to continue on the next line. The next line is concatenated to the previous line by removing the "&" character and line break. This allows long commands to be continued across two or more lines. See the discussion of triple quotes in *6* for how to continue a command across multiple line without using "&" characters.

2. All characters from the first "#" character onward are treated as comment and discarded. The exception to this rule is described in *6*. Note that a comment after a trailing "&" character will prevent the command from continuing on the next line. Also note that for multi-line commands a single leading "#" will comment out the entire command.

```
# this is a comment
timestep  1.0   # this is also a comment
```

3. The line is searched repeatedly for $ characters, which indicate variables that are replaced with a text string. The exception to this rule is described in *6*.

   If the $ is followed by text in curly brackets '{}', then the variable name is the text inside the curly brackets. If no curly brackets follow the $, then the variable name is the single character immediately following the $. Thus ${myTemp} and $x refer to variables named "myTemp" and "x", while "$xx" will be interpreted as a variable named "x" followed by an "x" character.

   How the variable is converted to a text string depends on what style of variable it is; see the *variable* doc page for details. It can be a variable that stores multiple text strings, and return one of them. The returned text string can be multiple "words" (space separated) which will then be interpreted as multiple arguments in the input command. The variable can also store a numeric formula which will be evaluated and its numeric result returned as a string.

   As a special case, if the $ is followed by parenthesis "()", then the text inside the parenthesis is treated as an "immediate" variable and evaluated as an *equal-style variable*. This is a way to use numeric formulas in an input script without having to assign them to variable names. For example, these 3 input script lines:

```
variable X equal (xlo+xhi)/2+sqrt(v_area)
region 1 block $X 2 INF INF EDGE EDGE
variable X delete
```

   can be replaced by:

```
region 1 block $((xlo+xhi)/2+sqrt(v_area)) 2 INF INF EDGE EDGE
```

   so that you do not have to define (or discard) a temporary variable, "X" in this case.

   Additionally, the "immediate" variable expression may be followed by a colon, followed by a C-style format string, e.g. ":%f" or ":%.10g". The format string must be appropriate for a double-precision floating-point value. The format string is used to output the result of the variable expression evaluation. If a format string is not specified a high-precision "%.20g" is used as the default.

   This can be useful for formatting print output to a desired precision:

```
print "Final energy per atom: $(pe/atoms:%10.3f) eV/atom"
```

Note that neither the curly-bracket or immediate form of variables can contain nested $ characters for other variables to substitute for. Thus you may **NOT** do this:

```
variable        a equal 2
variable        b2 equal 4
print           "B2 = ${b$a}"
```

Nor can you specify an expression like "$($x-1.0)" for an immediate variable, but you could use $(v_x-1.0), since the latter is valid syntax for an *equal-style variable*.

See the *variable* command for more details of how strings are assigned to variables and evaluated, and how they can be used in input script commands.

4. The line is broken into "words" separated by white-space (tabs, spaces). Note that words can thus contain letters, digits, underscores, or punctuation characters.

5. The first word is the command name. All successive words in the line are arguments.

6. If you want text with spaces to be treated as a single argument, it can be enclosed in either single or double or triple quotes. A long single argument enclosed in single or double quotes can span multiple lines if the "&" character is used, as described above. When the lines are concatenated together (and the "&" characters and line breaks removed), the text will become a single line. If you want multiple lines of an argument to retain their line breaks, the text can be enclosed in triple quotes, in which case "&" characters are not needed. For example:

```
print "Volume = $v"
print 'Volume = $v'
if "${steps} > 1000" then quit
variable a string "red green blue &
                 purple orange cyan"
print """
System volume = $v
System temperature = $t
"""
```

In each case, the single, double, or triple quotes are removed when the single argument they enclose is stored internally.

See the *dump modify format*, *print*, *if*, and *python* commands for examples.

A "#" or "$" character that is between quotes will not be treated as a comment indicator in *2* or substituted for as a variable in *3*.

Note: If the argument is itself a command that requires a quoted argument (e.g. using a *print* command as part of an *if* or *run every* command), then single, double, or triple quotes can be nested in the usual manner. See the doc pages for those commands for examples. Only one of level of nesting is allowed, but that should be sufficient for most use cases.

5.3 Input script structure

This page describes the structure of a typical LAMMPS input script. The examples directory in the LAMMPS distribution contains many sample input scripts; it is discussed on the *Examples* doc page.

A LAMMPS input script typically has 4 parts:

1. *Initialization*
2. *System definition*
3. *Simulation settings*
4. *Run a simulation*

The last 2 parts can be repeated as many times as desired. I.e. run a simulation, change some settings, run some more, etc. Each of the 4 parts is now described in more detail. Remember that almost all commands need only be used if a non-default value is desired.

5.3.1 Initialization

Set parameters that need to be defined before atoms are created or read-in from a file.

The relevant commands are *units*, *dimension*, *newton*, *processors*, *boundary*, *atom_style*, *atom_modify*.

If force-field parameters appear in the files that will be read, these commands tell LAMMPS what kinds of force fields are being used: *pair_style*, *bond_style*, *angle_style*, *dihedral_style*, *improper_style*.

5.3.2 System definition

There are 3 ways to define the simulation cell and reserve space for force field info and fill it with atoms in LAMMPS. Read them in from (1) a data file or (2) a restart file via the *read_data* or *read_restart* commands, respectively. These files can also contain molecular topology information. Or (3) create a simulation cell and fill it with atoms on a lattice (with no molecular topology), using these commands: *lattice*, *region*, *create_box*, *create_atoms* or *read_dump*.

The entire set of atoms can be duplicated to make a larger simulation using the *replicate* command.

5.3.3 Simulation settings

Once atoms and molecular topology are defined, a variety of settings can be specified: force field coefficients, simulation parameters, output options, and more.

Force field coefficients are set by these commands (they can also be set in the read-in files): *pair_coeff*, *bond_coeff*, *angle_coeff*, *dihedral_coeff*, *improper_coeff*, *kspace_style*, *dielectric*, *special_bonds*.

Various simulation parameters are set by these commands: *neighbor*, *neigh_modify*, *group*, *timestep*, *reset_timestep*, *run_style*, *min_style*, *min_modify*.

Fixes impose a variety of boundary conditions, time integration, and diagnostic options. The *fix* command comes in many flavors.

Various computations can be specified for execution during a simulation using the *compute*, *compute_modify*, and *variable* commands.

Output options are set by the *thermo*, *dump*, and *restart* commands.

5.3.4 Run a simulation

A molecular dynamics simulation is run using the *run* command. Energy minimization (molecular statics) is performed using the *minimize* command. A parallel tempering (replica-exchange) simulation can be run using the *temper* command.

5.4 Commands by category

This page lists most of the LAMMPS commands, grouped by category. The *General commands* doc page lists all general commands alphabetically. Style options for entries like fix, compute, pair etc. have their own pages where they are listed alphabetically.

5.4.1 Initialization:

newton	*package*	*processors*	*suffix*	*units*

5.4.2 Setup simulation box:

boundary	*box*	*change_box*	*create_box*
dimension	*lattice*	*region*	

5.4.3 Setup atoms:

atom_modify	*atom_style*	*balance*	*create_atoms*
create_bonds	*delete_atoms*	*delete_bonds*	*displace_atoms*
group	*mass*	*molecule*	*read_data*
read_dump	*read_restart*	*replicate*	*set*
velocity			

5.4.4 Force fields:

angle_coeff	*angle_style*	*bond_coeff*	*bond_style*
bond_write	*dielectric*	*dihedral_coeff*	*dihedral_style*
improper_coeff	*improper_style*	*kspace_modify*	*kspace_style*
pair_coeff	*pair_modify*	*pair_style*	*pair_write*
special_bonds			

5.4.5 Settings:

comm_modify	*comm_style*	*info*	*min_modify*
min_style	*neigh_modify*	*neighbor*	*partition*
reset_timestep	*run_style*	*timer*	*timestep*

5.4.6 Operations within timestepping (fixes) and diagnostics (computes):

compute	*compute_modify*	*fix*	*fix_modify*
uncompute	*unfix*		

5.4.7 Output:

dump image	*dump movie*	*dump*	*dump_modify*
restart	*thermo*	*thermo_modify*	*thermo_style*
undump	*write_coeff*	*write_data*	*write_dump*
write_restart			

5.4.8 Actions:

minimize	*neb*	*neb_spin*	*prd*	*rerun*	*run*
tad	*temper*				

5.4.9 Input script control:

clear	*echo*	*if*	*include*	*info*	*jump*	*label*
log	*next*	*print*	*python*	*quit*	*shell*	*variable*

General commands	*Fix styles*	*Compute styles*
Pair styles	*Bond styles*	*Angle styles*
Dihedral styles	*Improper styles*	*KSpace styles*

5.5 General commands

An alphabetic list of all general LAMMPS commands.

angle_coeff	*angle_style*	*atom_modify*	*atom_style*	*balance*
bond_coeff	*bond_style*	*bond_write*	*boundary*	*box*
change_box	*clear*	*comm_modify*	*comm_style*	*compute*
compute_modify	*create_atoms*	*create_bonds*	*create_box*	*delete_atoms*
delete_bonds	*dielectric*	*dihedral_coeff*	*dihedral_style*	*dimension*
displace_atoms	*dump*	*dump atom/adios*	*dump custom/adios*	*dump image*
dump movie	*dump netcdf*	*dump netcdf/mpiio*	*dump vtk*	*dump_modify*
dynamical_matrix	*echo*	*fix*	*fix_modify*	*group*
group2ndx	*hyper*	*if*	*improper_coeff*	*improper_style*
include	*info*	*jump*	*kim_init*	*kim_interactions*
kim_param	*kim_query*	*kspace_modify*	*kspace_style*	*label*
lattice	*log*	*mass*	*message*	*minimize*
min_modify	*min_style*	*min_style spin*	*molecule*	*ndx2group*
neb	*neb/spin*	*neigh_modify*	*neighbor*	*newton*
next	*package*	*pair_coeff*	*pair_modify*	*pair_write*
partition	*prd*	*print*	*processors*	*python*
quit	*read_data*	*read_dump*	*read_restart*	*region*
replicate	*rerun*	*reset_ids*	*reset_timestep*	*restart*
run	*run_style*	*server*	*set*	*shell*
special_bonds	*suffix*	*tad*	*temper*	*temper/grem*
temper/npt	*thermo*	*thermo_modify*	*thermo_style*	*third_order*
timer	*timestep*	*uncompute*	*undump*	*unfix*
units	*variable*	*velocity*	*write_coeff*	*write_data*
write_dump	*write_restart*			

General commands	*Fix styles*	*Compute styles*
Pair styles	*Bond styles*	*Angle styles*
Dihedral styles	*Improper styles*	*KSpace styles*

5.6 Fix commands

An alphabetic list of all LAMMPS *fix* commands. Some styles have accelerated versions. This is indicated by additional letters in parenthesis: g = GPU, i = USER-INTEL, k = KOKKOS, o = USER-OMP, t = OPT.

adapt	*adapt/fep*	*addforce*	*addtorque*	*append/atoms*
atc	*atom/swap*	*ave/atom*	*ave/chunk*	*ave/correlate*
ave/correlate/long	*ave/histo*	*ave/histo/weight*	*ave/time*	*aveforce*
balance	*bocs*	*bond/break*	*bond/create*	*bond/react*
bond/swap	*box/relax*	*client/md*	*cmap*	*colvars*
controller	*deform (k)*	*deposit*	*dpd/energy (k)*	*drag*
drude	*drude/transform/direct*	*drude/transform/inverse*	*dt/reset*	*edpd/source*
efield	*ehex*	*electron/stopping*	*enforce2d (k)*	*eos/cv*
eos/table	*eos/table/rx (k)*	*evaporate*	*external*	*ffl*
filter/corotate	*flow/gauss*	*freeze (k)*	*gcmc*	*gld*
gle	*gravity (ko)*	*grem*	*halt*	*heat*
hyper/global	*hyper/local*	*imd*	*indent*	*ipi*
langevin (k)	*langevin/drude*	*langevin/eff*	*langevin/spin*	*latte*
lb/fluid	*lb/momentum*	*lb/pc*	*lb/rigid/pc/sphere*	*lb/viscous*

Continued on next page

Table 1 – continued from previous page

lineforce	*manifoldforce*	*meso*	*meso/move*	*meso/stationary*
momentum (k)	*move*	*mscg*	*msst*	*mvv/dpd*
mvv/edpd	*mvv/tdpd*	*neb*	*neb/spin*	*nph (ko)*
nph/asphere (o)	*nph/body*	*nph/eff*	*nph/sphere (o)*	*nphug*
npt (iko)	*npt/asphere (o)*	*npt/body*	*npt/cauchy*	*npt/eff*
npt/sphere (o)	*npt/uef*	*nve (iko)*	*nve/asphere (i)*	*nve/asphere/noforce*
nve/awpmd	*nve/body*	*nve/dot*	*nve/dotc/langevin*	*nve/eff*
nve/limit	*nve/line*	*nve/manifold/rattle*	*nve/noforce*	*nve/sphere (ko)*
nve/spin	*nve/tri*	*nvk*	*nvt (iko)*	*nvt/asphere (o)*
nvt/body	*nvt/eff*	*nvt/manifold/rattle*	*nvt/sllod (io)*	*nvt/sllod/eff*
nvt/sphere (o)	*nvt/uef*	*oneway*	*orient/bcc*	*orient/fcc*
phonon	*pimd*	*planeforce*	*plumed*	*poems*
pour	*precession/spin*	*press/berendsen*	*print*	*propel/self*
property/atom (k)	*python/invoke*	*python/move*	*qbmsst*	*qeq/comb (o)*
qeq/dynamic	*qeq/fire*	*qeq/point*	*qeq/reax (ko)*	*qeq/shielded*
qeq/slater	*qmmm*	*qtb*	*rattle*	*reax/c/bonds (k)*
reax/c/species (k)	*recenter*	*restrain*	*rhok*	*rigid (o)*
rigid/meso	*rigid/nph (o)*	*rigid/nph/small*	*rigid/npt (o)*	*rigid/npt/small*
rigid/nve (o)	*rigid/nve/small*	*rigid/nvt (o)*	*rigid/nvt/small*	*rigid/small (o)*
rx (k)	*saed/vtk*	*setforce (k)*	*setforce/spin*	*shake*
shardlow (k)	*smd*	*smd/adjust_dt*	*smd/integrate_tlsph*	*smd/integrate_ulsph*
smd/move_tri_surf	*smd/setvel*	*smd/wall_surface*	*spring*	*spring/chunk*
spring/rg	*spring/self*	*srd*	*store/force*	*store/state*
tdpd/source	*temp/berendsen*	*temp/csld*	*temp/csvr*	*temp/rescale*
temp/rescale/eff	*tfmc*	*thermal/conductivity*	*ti/spring*	*tmd*
ttm	*ttm/mod*	*tune/kspace*	*vector*	*viscosity*
viscous	*wall/body/polygon*	*wall/body/polyhedron*	*wall/colloid*	*wall/ees*
wall/gran	*wall/gran/region*	*wall/harmonic*	*wall/lj1043*	*wall/lj126*
wall/lj93 (k)	*wall/morse*	*wall/piston*	*wall/reflect (k)*	*wall/reflect/stochastic*
wall/region	*wall/region/ees*	*wall/srd*		

General commands	*Fix styles*	*Compute styles*
Pair styles	*Bond styles*	*Angle styles*
Dihedral styles	*Improper styles*	*KSpace styles*

5.7 Compute commands

An alphabetic list of all LAMMPS *compute* commands. Some styles have accelerated versions. This is indicated by additional letters in parenthesis: g = GPU, i = USER-INTEL, k = KOKKOS, o = USER-OMP, t = OPT.

ackland/atom	*adf*	*aggregate/atom*	*angle*	*angle/local*
angmom/chunk	*basal/atom*	*body/local*	*bond*	*bond/local*
centro/atom	*centroid/stress/atom*	*chunk/atom*	*chunk/spread/atom*	*cluster/atom*
cna/atom	*cnp/atom*	*com*	*com/chunk*	*contact/atom*
coord/atom	*damage/atom*	*dihedral*	*dihedral/local*	*dilatation/atom*
dipole/chunk	*displace/atom*	*dpd*	*dpd/atom*	*edpd/temp/atom*
entropy/atom	*erotate/asphere*	*erotate/rigid*	*erotate/sphere*	*erotate/sphere/atom*
event/displace	*fep*	*force/tally*	*fragment/atom*	*global/atom*
group/group	*gyration*	*gyration/chunk*	*gyration/shape*	*gyration/shape/chunk*
heat/flux	*heat/flux/tally*	*hexorder/atom*	*hma*	*improper*
improper/local	*inertia/chunk*	*ke*	*ke/atom*	*ke/atom/eff*
ke/eff	*ke/rigid*	*meso/e/atom*	*meso/rho/atom*	*meso/t/atom*
momentum	*msd*	*msd/chunk*	*msd/nongauss*	*omega/chunk*
orientorder/atom	*pair*	*pair/local*	*pe*	*pe/atom*
pe/mol/tally	*pe/tally*	*plasticity/atom*	*pressure*	*pressure/cylinder*
pressure/uef	*property/atom*	*property/chunk*	*property/local*	*ptm/atom*
rdf	*reduce*	*reduce/chunk*	*reduce/region*	*rigid/local*
saed	*slice*	*smd/contact/radius*	*smd/damage*	*smd/hourglass/error*
smd/internal/energy	*smd/plastic/strain*	*smd/plastic/strain/rate*	*smd/rho*	*smd/tlsph/defgrad*
smd/tlsph/dt	*smd/tlsph/num/neighs*	*smd/tlsph/shape*	*smd/tlsph/strain*	*smd/tlsph/strain/rate*
smd/tlsph/stress	*smd/triangle/vertices*	*smd/ulsph/num/neighs*	*smd/ulsph/strain*	*smd/ulsph/strain/rate*
smd/ulsph/stress	*smd/vol*	*snap*	*sna/atom*	*snad/atom*
snav/atom	*spin*	*stress/atom*	*stress/mop*	*stress/mop/profile*
stress/tally	*tdpd/cc/atom*	*temp (k)*	*temp/asphere*	*temp/body*
temp/chunk	*temp/com*	*temp/cs*	*temp/deform*	*temp/deform/eff*
temp/drude	*temp/eff*	*temp/partial*	*temp/profile*	*temp/ramp*
temp/region	*temp/region/eff*	*temp/rotate*	*temp/sphere*	*temp/uef*
ti	*torque/chunk*	*vacf*	*vcm/chunk*	*voronoi/atom*
xrd				

General commands	*Fix styles*	*Compute styles*
Pair styles	*Bond styles*	*Angle styles*
Dihedral styles	*Improper styles*	*KSpace styles*

5.8 Pair_style potentials

All LAMMPS *pair_style* commands. Some styles have accelerated versions. This is indicated by additional letters in parenthesis: g = GPU, i = USER-INTEL, k = KOKKOS, o = USER-OMP, t = OPT.

none	*zero*	*hybrid (k)*	*hybrid/overlay (k)*
kim	*list*		
adp (o)	*agni (o)*	*airebo (io)*	*airebo/morse (io)*
atm	*awpmd/cut*	*beck (go)*	*body/nparticle*
body/rounded/polygon	*body/rounded/polyhedron*	*bop*	*born (go)*
born/coul/dsf	*born/coul/dsf/cs*	*born/coul/long (go)*	*born/coul/long/cs (g)*
born/coul/msm (o)	*born/coul/wolf (go)*	*born/coul/wolf/cs (g)*	*brownian (o)*

Continued on next page

Table 2 – continued from previous page

brownian/poly (o)	*buck (giko)*	*buck/coul/cut (giko)*	*buck/coul/long (giko)*
buck/coul/long/cs	*buck/coul/msm (o)*	*buck/long/coul/long (o)*	*buck/mdf*
buck6d/coul/gauss/dsf	*buck6d/coul/gauss/long*	*colloid (go)*	*comb (o)*
comb3	*cosine/squared*	*coul/cut (gko)*	*coul/cut/soft (o)*
coul/debye (gko)	*coul/diel (o)*	*coul/dsf (gko)*	*coul/long (gko)*
coul/long/cs (g)	*coul/long/soft (o)*	*coul/msm (o)*	*coul/shield*
coul/streitz	*coul/wolf (ko)*	*coul/wolf/cs*	*dpd (gio)*
dpd/fdt	*dpd/fdt/energy (k)*	*dpd/tstat (go)*	*dsmc*
e3b	*drip*	*eam (gikot)*	*eam/alloy (gikot)*
eam/cd (o)	*eam/cd/old (o)*	*eam/fs (gikot)*	*edip (o)*
edip/multi	*edpd*	*eff/cut*	*eim (o)*
exp6/rx (k)	*extep*	*gauss (go)*	*gauss/cut (o)*
gayberne (gio)	*gran/hertz/history (o)*	*gran/hooke (o)*	*gran/hooke/history (ko)*
granular	*gw*	*gw/zbl*	*hbond/dreiding/lj (o)*
hbond/dreiding/morse (o)	*ilp/graphene/hbn*	*kolmogorov/crespi/full*	*kolmogorov/crespi/z*
lcbop	*lebedeva/z*	*lennard/mdf*	*line/lj*
lj/charmm/coul/charmm (iko)	*lj/charmm/coul/charmm/implicit (ko)*	*lj/charmm/coul/long (gikot)*	*lj/charmm/coul/long/soft (o)*
lj/charmm/coul/msm (o)	*lj/charmmfsw/coul/charmmfsh*	*lj/charmmfsw/coul/long*	*lj/class2 (gko)*
lj/class2/coul/cut (ko)	*lj/class2/coul/cut/soft*	*lj/class2/coul/long (gko)*	*lj/class2/coul/long/soft*
lj/class2/soft	*lj/cubic (go)*	*lj/cut (gikot)*	*lj/cut/coul/cut (gko)*
lj/cut/coul/cut/soft (o)	*lj/cut/coul/debye (gko)*	*lj/cut/coul/dsf (gko)*	*lj/cut/coul/long (gikot)*
lj/cut/coul/long/cs	*lj/cut/coul/long/soft (o)*	*lj/cut/coul/msm (go)*	*lj/cut/coul/wolf (o)*
lj/cut/dipole/cut (go)	*lj/cut/dipole/long (g)*	*lj/cut/dipole/sf (go)*	*lj/cut/soft (o)*
lj/cut/thole/long (o)	*lj/cut/tip4p/cut (o)*	*lj/cut/tip4p/long (got)*	*lj/cut/tip4p/long/soft (o)*
lj/expand (gko)	*lj/expand/coul/long (g)*	*lj/gromacs (gko)*	*lj/gromacs/coul/gromacs (ko)*
lj/long/coul/long (iot)	*lj/long/dipole/long*	*lj/long/tip4p/long (o)*	*lj/mdf*
lj/sdk (gko)	*lj/sdk/coul/long (go)*	*lj/sdk/coul/msm (o)*	*lj/sf/dipole/sf (go)*
lj/smooth (o)	*lj/smooth/linear (o)*	*lj/switch3/coulgauss/long*	*lj96/cut (go)*
local/density	*lubricate (o)*	*lubricate/poly (o)*	*lubricateU*
lubricateU/poly	*mdpd*	*mdpd/rhosum*	*meam/c*
meam/spline (o)	*meam/sw/spline*	*mesocnt*	*mgpt*
mie/cut (g)	*mm3/switch3/coulgauss/long*	*momb*	*morse (gkot)*
morse/smooth/linear (o)	*morse/soft*	*multi/lucy*	*multi/lucy/rx (k)*
nb3b/harmonic	*nm/cut (o)*	*nm/cut/coul/cut (o)*	*nm/cut/coul/long (o)*
oxdna/coaxstk	*oxdna/excv*	*oxdna/hbond*	*oxdna/stk*
oxdna/xstk	*oxdna2/coaxstk*	*oxdna2/dh*	*oxdna2/excv*
oxdna2/hbond	*oxdna2/stk*	*oxdna2/xstk*	*oxrna2/excv*
oxrna2/hbond	*oxrna2/dh*	*oxrna2/stk*	*oxrna2/xstk*
oxrna2/coaxstk	*peri/eps*	*peri/lps (o)*	*peri/pmb (o)*
peri/ves	*polymorphic*	*python*	*quip*
reax/c (ko)	*rebo (io)*	*resquared (go)*	*sdpd/taitwater/isothermal*
smd/hertz	*smd/tlsph*	*smd/tri_surface*	*smd/ulsph*
smtbq	*snap (k)*	*snap (k)*	*soft (go)*
sph/heatconduction	*sph/idealgas*	*sph/lj*	*sph/rhosum*
sph/taitwater	*sph/taitwater/morris*	*spin/dipole/cut*	*spin/dipole/long*
spin/dmi	*spin/exchange*	*spin/magelec*	*spin/neel*
srp	*sw (giko)*	*table (gko)*	*table/rx (k)*
tdpd	*tersoff (giko)*	*tersoff/mod (gko)*	*tersoff/mod/c (o)*
tersoff/table (o)	*tersoff/zbl (gko)*	*thole*	*tip4p/cut (o)*
tip4p/long (o)	*tip4p/long/soft (o)*	*tri/lj*	*ufm (got)*

Continued on next page

Table 2 – continued from previous page

vashishta (gko)	*vashishta/table (o)*	*yukawa (gko)*	*yukawa/colloid (go)*
zbl (gko)			

General commands	*Fix styles*	*Compute styles*
Pair styles	*Bond styles*	*Angle styles*
Dihedral styles	*Improper styles*	*KSpace styles*

5.9 Bond_style potentials

All LAMMPS *bond_style* commands. Some styles have accelerated versions. This is indicated by additional letters in parenthesis: g = GPU, i = USER-INTEL, k = KOKKOS, o = USER-OMP, t = OPT.

none	*zero*	*hybrid*	
class2 (ko)	*fene (iko)*	*fene/expand (o)*	*gromos (o)*
harmonic (iko)	*harmonic/shift (o)*	*harmonic/shift/cut (o)*	*mm3*
morse (o)	*nonlinear (o)*	*oxdna/fene*	*oxdna2/fene*
oxrna2/fene	*quartic (o)*	*table (o)*	

5.10 Angle_style potentials

All LAMMPS *angle_style* commands. Some styles have accelerated versions. This is indicated by additional letters in parenthesis: g = GPU, i = USER-INTEL, k = KOKKOS, o = USER-OMP, t = OPT.

none	*zero*	*hybrid*	
charmm (iko)	*class2 (ko)*	*class2/p6*	*cosine (ko)*
cosine/buck6d	*cosine/delta (o)*	*cosine/periodic (o)*	*cosine/shift (o)*
cosine/shift/exp (o)	*cosine/squared (o)*	*cross*	*dipole (o)*
fourier (o)	*fourier/simple (o)*	*harmonic (iko)*	*mm3*
quartic (o)	*sdk (o)*	*table (o)*	

5.11 Dihedral_style potentials

All LAMMPS *dihedral_style* commands. Some styles have accelerated versions. This is indicated by additional letters in parenthesis: g = GPU, i = USER-INTEL, k = KOKKOS, o = USER-OMP, t = OPT.

none	*zero*	*hybrid*	
charmm (iko)	*charmmfsw*	*class2 (ko)*	*cosine/shift/exp (o)*
fourier (io)	*harmonic (iko)*	*helix (o)*	*multi/harmonic (o)*
nharmonic (o)	*opls (iko)*	*quadratic (o)*	*spherical*
table (o)	*table/cut*		

5.12 Improper_style potentials

All LAMMPS *improper_style* commands. Some styles have accelerated versions. This is indicated by additional letters in parenthesis: g = GPU, i = USER-INTEL, k = KOKKOS, o = USER-OMP, t = OPT.

none	*zero*	*hybrid*	
class2 (ko)	*cossq (o)*	*cvff (io)*	*distance*
distharm	*fourier (o)*	*harmonic (iko)*	*inversion/harmonic*
ring (o)	*sqdistharm*	*umbrella (o)*	

General commands	*Fix styles*	*Compute styles*
Pair styles	*Bond styles*	*Angle styles*
Dihedral styles	*Improper styles*	*KSpace styles*

5.13 KSpace solvers

All LAMMPS *kspace_style* solvers. Some styles have accelerated versions. This is indicated by additional letters in parenthesis: g = GPU, i = USER-INTEL, k = KOKKOS, o = USER-OMP, t = OPT.

ewald (o)	*ewald/disp*	*ewald/dipole*	*ewald/dipole/spin*
msm (o)	*msm/cg (o)*	*pppm (giko)*	*pppm/cg (o)*
pppm/dipole	*pppm/dipole/spin*	*pppm/disp (io)*	*pppm/disp/tip4p (o)*
pppm/stagger	*pppm/tip4p (o)*	*scafacos*	

5.14 Removed commands and packages

This page lists LAMMPS commands and packages that have been removed from the distribution and provides suggestions for alternatives or replacements. LAMMPS has special dummy styles implemented, that will stop LAMMPS and print a suitable error message in most cases, when a style/command is used that has been removed.

5.14.1 Fix ave/spatial and fix ave/spatial/sphere

The fixes ave/spatial and ave/spatial/sphere have been removed from LAMMPS since they were superseded by the more general and extensible "chunk infrastructure". Here the system is partitioned in one of many possible ways through the *compute chunk/atom* command and then averaging is done using *fix ave/chunk*. Please refer to the *chunk HOWTO* section for an overview.

5.14.2 MEAM package

The MEAM package has been removed since it was superseded by the *USER-MEAMC package*. The code in the USER-MEAMC package is a translation of the Fortran code of MEAM into C++, which removes several restrictions (e.g. there can be multiple instances in hybrid pair styles) and allows for some optimizations leading to better performance. The new pair style *meam/c* has the exact same syntax as the old "meam" pair style and thus pair style *meam* is an alias to the new style and backward compatibility of old inputs is preserved.

5.14.3 REAX package

The REAX package has been removed since it was superseded by the *USER-REAXC package*. The USER-REAXC package has been tested to yield equivalent results to the REAX package, offers better performance, supports OpenMP multi-threading via USER-OMP, and GPU and threading parallelization through KOKKOS. The new pair styles are not syntax compatible with the removed reax pair style, so input files will have to be adapted.

5.14.4 USER-CUDA package

The USER-CUDA package had been removed, since it had been unmaintained for a long time and had known bugs and problems. Significant parts of the design were transferred to the *KOKKOS package*, which has similar performance characteristics on Nvidia GPUs. Both, the KOKKOS and the *GPU package* are maintained and allow running LAMMPS with GPU acceleration.

5.14.5 restart2data tool

The functionality of the restart2data tool has been folded into the LAMMPS executable directly instead of having a separate tool. A combination of the commands *read_restart* and *write_data* can be used to the same effect. For added convenience this conversion can also be triggered by *command line flags*

CHAPTER

SIX

OPTIONAL PACKAGES

This section gives an overview of the optional packages that extend LAMMPS functionality. Packages are groups of files that enable a specific set of features. For example, force fields for molecular systems or rigid-body constraints are in packages. You can see the list of all packages and "make" commands to manage them by typing "make package" from within the src directory of the LAMMPS distribution. The *Build package* doc page gives general info on how to install and un-install packages as part of the LAMMPS build process.

6.1 Standard packages

This is the list of standard packages in LAMMPS. The link for each package name gives more details.

Standard packages are supported by the LAMMPS developers and are written in a syntax and style consistent with the rest of LAMMPS. This means the developers will answer questions about them, debug and fix them if necessary, and keep them compatible with future changes to LAMMPS.

The "Example" column is a sub-directory in the examples directory of the distribution which has an input script that uses the package. E.g. "peptide" refers to the examples/peptide directory; USER/atc refers to the examples/USER/atc directory. The "Library" column indicates whether an extra library is needed to build and use the package:

- no = no library
- sys = system library: you likely have it on your machine
- int = internal library: provided with LAMMPS, but you may need to build it
- ext = external library: you will need to download and install it on your machine

Package	Description	Doc page	Example	Library
ASPHERE	aspherical particle models	*Howto spherical*	ellipse	no
BODY	body-style particles	*Howto body*	body	no
CLASS2	class 2 force fields	*pair_style lj/class2*	n/a	no
COLLOID	colloidal particles	*atom_style colloid*	colloid	no
COMPRESS	I/O compression	*dump */gz*	n/a	sys
CORESHELL	adiabatic core/shell model	*Howto coreshell*	coreshell	no
DIPOLE	point dipole particles	*pair_style dipole/cut*	dipole	no
GPU	GPU-enabled styles	*Section gpu*	Benchmarks	int
GRANULAR	granular systems	*Howto granular*	pour	no
KIM	OpenKIM wrapper	*pair_style kim*	kim	ext
KOKKOS	Kokkos-enabled styles	*Speed kokkos*	Benchmarks	no
KSPACE	long-range Coulombic solvers	*kspace_style*	peptide	no
LATTE	quantum DFTB forces via LATTE	*fix latte*	latte	ext
MANYBODY	many-body potentials	*pair_style tersoff*	shear	no

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Table 1 – continued from previous page

MC	Monte Carlo options	*fix gcmc*	n/a	no
MESSAGE	client/server messaging	*message*	message	int
MISC	miscellaneous single-file commands	n/a	no	no
MOLECULE	molecular system force fields	*Howto bioFF*	peptide	no
MPIIO	MPI parallel I/O dump and restart	*dump*	n/a	no
MSCG	multi-scale coarse-graining wrapper	*fix mscg*	mscg	ext
OPT	optimized pair styles	*Speed opt*	Benchmarks	no
PERI	Peridynamics models	*pair_style peri*	peri	no
POEMS	coupled rigid body motion	*fix poems*	rigid	int
PYTHON	embed Python code in an input script	*python*	python	sys
QEQ	QEq charge equilibration	*fix qeq*	qeq	no
REPLICA	multi-replica methods	*Howto replica*	tad	no
RIGID	rigid bodies and constraints	*fix rigid*	rigid	no
SHOCK	shock loading methods	*fix msst*	n/a	no
SNAP	quantum-fitted potential	*pair_style snap*	snap	no
SPIN	magnetic atomic spin dynamics	*Howto spins*	SPIN	no
SRD	stochastic rotation dynamics	*fix srd*	srd	no
VORONOI	Voronoi tesselation	*compute voronoi/atom*	n/a	ext

6.2 User packages

This is a list of user packages in LAMMPS. The link for each package name gives more details.

User packages have been contributed by users, and begin with the "user" prefix. If a contribution is a single command (single file), it is typically in the user-misc package. User packages don't necessarily meet the requirements of the *standard packages*. This means the developers will try to keep things working and usually can answer technical questions about compiling the package. If you have problems using a specific feature provided in a user package, you may need to contact the contributor directly to get help. Information on how to submit additions you make to LAMMPS as single files or as a standard or user package is explained on the *Modify contribute* doc page.

The "Example" column is a sub-directory in the examples directory of the distribution which has an input script that uses the package. E.g. "peptide" refers to the examples/peptide directory; USER/atc refers to the examples/USER/atc directory. The "Library" column indicates whether an extra library is needed to build and use the package:

- no = no library
- sys = system library: you likely have it on your machine
- int = internal library: provided with LAMMPS, but you may need to build it
- ext = external library: you will need to download and install it on your machine

Package	Description	Doc page	Example	L
USER-ADIOS	dump output via ADIOS	*dump adios*	USER/adios	e
USER-ATC	Atom-to-Continuum coupling	*fix atc*	USER/atc	i
USER-AWPMD	wave packet MD	*pair_style awpmd/cut*	USER/awpmd	i
USER-BOCS	BOCS bottom up coarse graining	*fix bocs*	USER/bocs	n
USER-CGDNA	coarse-grained DNA force fields	src/USER-CGDNA/README	USER/cgdna	n
USER-CGSDK	SDK coarse-graining model	*pair_style lj/sdk*	USER/cgsdk	n
USER-COLVARS	collective variables library	*fix colvars*	USER/colvars	i
USER-DIFFRACTION	virtual x-ray and electron diffraction	*compute xrd*	USER/diffraction	n
USER-DPD	reactive dissipative particle dynamics	src/USER-DPD/README	USER/dpd	n

Continued on nex

Table 2 – continued from previous page

USER-DRUDE	Drude oscillators	*Howto drude*	USER/drude	n
USER-EFF	electron force field	*pair_style eff/cut*	USER/eff	n
USER-FEP	free energy perturbation	*compute fep*	USER/fep	n
USER-H5MD	dump output via HDF5	*dump h5md*	n/a	e
USER-INTEL	optimized Intel CPU and KNL styles	*Speed intel*	Benchmarks	n
USER-LB	Lattice Boltzmann fluid	*fix lb/fluid*	USER/lb	n
USER-MANIFOLD	motion on 2d surfaces	*fix manifoldforce*	USER/manifold	n
USER-MEAMC	modified EAM potential (C++)	*pair_style meam/c*	meamc	n
USER-MESO	mesoscale DPD models	*pair_style edpd*	USER/meso	n
USER-MGPT	fast MGPT multi-ion potentials	*pair_style mgpt*	USER/mgpt	n
USER-MISC	single-file contributions	USER-MISC/README	USER/misc	n
USER-MOFFF	styles for MOF-FF force field	*pair_style buck6d/coul/gauss*	USER/mofff	n
USER-MOLFILE	VMD molfile plug-ins	*dump molfile*	n/a	e
USER-NETCDF	dump output via NetCDF	*dump netcdf*	n/a	e
USER-OMP	OpenMP-enabled styles	*Speed omp*	Benchmarks	n
USER-PHONON	phonon dynamical matrix	*fix phonon*	USER/phonon	n
USER-PLUMED	*PLUMED* free energy library	*fix plumed*	USER/plumed	e
USER-PTM	Polyhedral Template Matching	*compute ptm/atom*	n/a	n
USER-QMMM	QM/MM coupling	*fix qmmm*	USER/qmmm	e
USER-QTB	quantum nuclear effects	*fix qtb fix qbmsst*	qtb	n
USER-QUIP	QUIP/libatoms interface	*pair_style quip*	USER/quip	e
USER-REAXC	ReaxFF potential (C/C++)	*pair_style reaxc*	reax	n
USER-SCAFACOS	wrapper on ScaFaCoS solver	*kspace_style scafacos*	USER/scafacos	e
USER-SDPD	smoothed dissipative particle dynamics	*pair_style sdpd/taitwater/isothermal*	USER/sdpd	n
USER-SMD	smoothed Mach dynamics	SMD User Guide	USER/smd	e
USER-SMTBQ	second moment tight binding QEq potential	*pair_style smtbq*	USER/smtbq	n
USER-SPH	smoothed particle hydrodynamics	SPH User Guide	USER/sph	n
USER-TALLY	pairwise tally computes	*compute XXX/tally*	USER/tally	n
USER-UEF	extensional flow	*fix nvt/uef*	USER/uef	n
USER-VTK	dump output via VTK	*compute vtk*	n/a	e
USER-YAFF	additional styles implemented in YAFF	*angle_style cross*	USER/yaff	n

6.3 Package details

Here is a brief description of all the standard and user packages in LAMMPS. It lists authors (if applicable) and summarizes the package contents. It has specific instructions on how to install the package, including, if necessary, info on how to download or build any extra library it requires. It also gives links to documentation, example scripts, and pictures/movies (if available) that illustrate use of the package.

The majority of packages can be included in a LAMMPS build with a single setting (-D PGK_NAME for CMake) or command ("make yes-name" for make). See the *Build package* doc page for more info. A few packages may require additional steps; this is indicated in the descriptions below. The *Build extras* doc page gives those details.

Note: To see the complete list of commands a package adds to LAMMPS, you can examine the files in its src directory, e.g. "ls src/GRANULAR". Files with names that start with fix, compute, atom, pair, bond, angle, etc correspond to commands with the same style name as contained in the file name.

ASPHERE	*BODY*	*CLASS2*	*COLLOID*	*COMPRESS*	*CORESHELL*
DIPOLE	*GPU*	*GRANULAR*	*KIM*	*KOKKOS*	*KSPACE*
LATTE	*MANYBODY*	*MC*	*MESSAGE*	*MISC*	*MOLECULE*
MPIIO	*MSCG*	*OPT*	*PERI*	*POEMS*	*PYTHON*
QEQ	*REPLICA*	*RIGID*	*SHOCK*	*SNAP*	*SPIN*
SRD	*VORONOI*				

USER-ADIOS	*USER-ATC*	*USER-AWPMD*	*USER-BOCS*	*USER-CGDNA*	*USER-CGSDK*
USER-COLVARS	*USER-DIFFRACTION*	*USER-DPD*	*USER-DRUDE*	*USER-EFF*	*USER-FEP*
USER-H5MD	*USER-INTEL*	*USER-LB*	*USER-MANIFOLD*	*USER-MEAMC*	*USER-MESO*
USER-MGPT	*USER-MISC*	*USER-MOFFF*	*USER-MOLFILE*	*USER-NETCDF*	*USER-OMP*
USER-PHONON	*USER-PLUMED*	*USER-PTM*	*USER-QMMM*	*USER-QTB*	*USER-QUIP*
USER-REAXC	*USER-SCAFACOS*	*USER-SDPD*	*USER-SMD*	*USER-SMTBQ*	*USER-SPH*
USER-TALLY	*USER-UEF*	*USER-VTK*	*USER-YAFF*		

6.3.1 ASPHERE package

Contents:

Computes, time-integration fixes, and pair styles for aspherical particle models including ellipsoids, 2d lines, and 3d triangles.

Supporting info:

- src/ASPHERE: filenames -> commands
- *Howto spherical*
- *pair_style gayberne*
- *pair_style resquared*
- doc/PDF/pair_gayberne_extra.pdf
- doc/PDF/pair_resquared_extra.pdf
- examples/ASPHERE
- examples/ellipse
- http://lammps.sandia.gov/movies.html#line
- http://lammps.sandia.gov/movies.html#tri

6.3.2 BODY package

Contents:

Body-style particles with internal structure. Computes, time-integration fixes, pair styles, as well as the body styles themselves. See the *Howto body* doc page for an overview.

Supporting info:

- src/BODY filenames -> commands
- *Howto_body*
- *atom_style body*
- *fix nve/body*
- *pair_style body/nparticle*
- examples/body

6.3.3 CLASS2 package

Contents:

Bond, angle, dihedral, improper, and pair styles for the COMPASS CLASS2 molecular force field.

Supporting info:

- src/CLASS2: filenames -> commands
- *bond_style class2*
- *angle_style class2*
- *dihedral_style class2*
- *improper_style class2*
- *pair_style lj/class2*

6.3.4 COLLOID package

Contents:

Coarse-grained finite-size colloidal particles. Pair styles and fix wall styles for colloidal interactions. Includes the Fast Lubrication Dynamics (FLD) method for hydrodynamic interactions, which is a simplified approximation to Stokesian dynamics.

Authors: This package includes Fast Lubrication Dynamics pair styles which were created by Amit Kumar and Michael Bybee from Jonathan Higdon's group at UIUC.

Supporting info:

- src/COLLOID: filenames -> commands
- *fix wall/colloid*
- *pair_style colloid*

- *pair_style yukawa/colloid*
- *pair_style brownian*
- *pair_style lubricate*
- *pair_style lubricateU*
- examples/colloid
- examples/srd

6.3.5 COMPRESS package

Contents:

Compressed output of dump files via the zlib compression library, using dump styles with a "gz" in their style name.

To use this package you must have the zlib compression library available on your system.

Author: Axel Kohlmeyer (Temple U).

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/COMPRESS: filenames -> commands
- src/COMPRESS/README
- lib/compress/README
- *dump atom/gz*
- *dump cfg/gz*
- *dump custom/gz*
- *dump xyz/gz*

6.3.6 CORESHELL package

Contents:

Compute and pair styles that implement the adiabatic core/shell model for polarizability. The pair styles augment Born, Buckingham, and Lennard-Jones styles with core/shell capabilities. The *compute temp/cs* command calculates the temperature of a system with core/shell particles. See the *Howto coreshell* doc page for an overview of how to use this package.

Author: Hendrik Heenen (Technical U of Munich).

Supporting info:

- src/CORESHELL: filenames -> commands
- *Howto coreshell*
- *Howto polarizable*

- *compute temp/cs*
- *pair_style born/coul/long/cs*
- *pair_style buck/coul/long/cs*
- *pair_style lj/cut/coul/long/cs*
- examples/coreshell

6.3.7 DIPOLE package

Contents:

An atom style and several pair styles for point dipole models with short-range or long-range interactions.

Supporting info:

- src/DIPOLE: filenames -> commands
- *atom_style dipole*
- *pair_style lj/cut/dipole/cut*
- *pair_style lj/cut/dipole/long*
- *pair_style lj/long/dipole/long*
- examples/dipole

6.3.8 GPU package

Contents:

Dozens of pair styles and a version of the PPPM long-range Coulombic solver optimized for GPUs. All such styles have a "gpu" as a suffix in their style name. The GPU code can be compiled with either CUDA or OpenCL, however the OpenCL variants are no longer actively maintained and only the CUDA versions are regularly tested. The *Speed gpu* doc page gives details of what hardware and GPU software is required on your system, and details on how to build and use this package. Its styles can be invoked at run time via the "-sf gpu" or "-suffix gpu" *command-line switches*. See also the *KOKKOS* package, which has GPU-enabled styles.

Authors: Mike Brown (Intel) while at Sandia and ORNL and Trung Nguyen (Northwestern U) while at ORNL.

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/GPU: filenames -> commands
- src/GPU/README
- lib/gpu/README
- *Speed packages*
- *Speed gpu*
- *Section 2.6 -sf gpu*

- *Section 2.6 -pk gpu*
- *package gpu*
- *Commands* pages (*pair*, *kspace*) for styles followed by (g)
- Benchmarks page of web site

6.3.9 GRANULAR package

Contents:

Pair styles and fixes for finite-size granular particles, which interact with each other and boundaries via frictional and dissipative potentials.

Supporting info:

- src/GRANULAR: filenames -> commands
- *Howto granular*
- *fix pour*
- *fix wall/gran*
- *pair_style gran/hooke*
- *pair_style gran/hertz/history*
- examples/granregion
- examples/pour
- bench/in.chute
- http://lammps.sandia.gov/pictures.html#jamming
- http://lammps.sandia.gov/movies.html#hopper
- http://lammps.sandia.gov/movies.html#dem
- http://lammps.sandia.gov/movies.html#brazil
- http://lammps.sandia.gov/movies.html#granregion

6.3.10 KIM package

Contents:

This package contains a set of commands that serve as a wrapper on the Open Knowledgebase of Interatomic Models (OpenKIM) repository of interatomic models (IMs) enabling compatible ones to be used in LAMMPS simulations. This includes *kim_init and kim_interactions* commands to select, initialize and instantiate the IM, and a *kim_query* command to perform web queries for material property predictions of OpenKIM IMs. Support for KIM IMs that conform to the KIM Application Programming Interface (API) is provided by the *pair_style kim* command.

Note: The command *pair_style kim* is called by *kim_interactions* and is not recommended to be directly used in input scripts.

To use this package you must have the KIM API library available on your system. The KIM API is available for download on the OpenKIM website. When installing LAMMPS from binary, the kim-api package is a dependency that is automatically downloaded and installed.

Information about the KIM project can be found at its website: https://openkim.org. The KIM project is led by Ellad Tadmor and Ryan Elliott (U Minnesota) and is funded by the National Science Foundation.

Authors: Ryan Elliott (U Minnesota) is the main developer for the KIM API and the *pair_style kim* command. Axel Kohlmeyer (Temple U) and Ellad Tadmor (U Minnesota) contributed to the *kim_commands* interface in close collaboration with Ryan Elliott.

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- *kim_commands*
- *pair_style kim*
- src/KIM: filenames -> commands
- src/KIM/README
- lib/kim/README
- examples/kim

6.3.11 KOKKOS package

Contents:

Dozens of atom, pair, bond, angle, dihedral, improper, fix, compute styles adapted to compile using the Kokkos library which can convert them to OpenMP or CUDA code so that they run efficiently on multicore CPUs, KNLs, or GPUs. All the styles have a "kk" as a suffix in their style name. The *Speed kokkos* doc page gives details of what hardware and software is required on your system, and how to build and use this package. Its styles can be invoked at run time via the "-sf kk" or "-suffix kk" *command-line switches*. Also see the *GPU*, *OPT*, *USER-INTEL*, and *USER-OMP* packages, which have styles optimized for CPUs, KNLs, and GPUs.

You must have a C++11 compatible compiler to use this package. KOKKOS makes extensive use of advanced C++ features, which can expose compiler bugs, especially when compiling for maximum performance at high optimization levels. Please see the file lib/kokkos/README for a list of compilers and their respective platforms, that are known to work.

Authors: The KOKKOS package was created primarily by Christian Trott and Stan Moore (Sandia), with contributions from other folks as well. It uses the open-source Kokkos library which was developed by Carter Edwards, Christian Trott, and others at Sandia, and which is included in the LAMMPS distribution in lib/kokkos.

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/KOKKOS: filenames -> commands
- src/KOKKOS/README
- lib/kokkos/README
- *Speed packages*

- *Speed kokkos*
- *Section 2.6 -k on . . .*
- *Section 2.6 -sf kk*
- *Section 2.6 -pk kokkos*
- *package kokkos*
- Search the *commands* pages (*fix*, *compute*, *pair*, *bond, angle, dihedral, improper*, *kspace*) for styles followed by (k)
- Benchmarks page of web site

6.3.12 KSPACE package

Contents:

A variety of long-range Coulombic solvers, as well as pair styles which compute the corresponding short-range pairwise Coulombic interactions. These include Ewald, particle-particle particle-mesh (PPPM), and multilevel summation method (MSM) solvers.

Install:

Building with this package requires a 1d FFT library be present on your system for use by the PPPM solvers. This can be the KISS FFT library provided with LAMMPS, 3rd party libraries like FFTW, or a vendor-supplied FFT library. See the *Build settings* doc page for details on how to select different FFT options for your LAMPMS build.

Supporting info:

- src/KSPACE: filenames -> commands
- *kspace_style*
- doc/PDF/kspace.pdf
- *Howto tip3p*
- *Howto tip4p*
- *Howto spc*
- *pair_style coul*
- Search the *pair style* page for styles with "long" or "msm" in name
- examples/peptide
- bench/in.rhodo

6.3.13 LATTE package

Contents:

A fix command which wraps the LATTE DFTB code, so that molecular dynamics can be run with LAMMPS using density-functional tight-binding quantum forces calculated by LATTE.

More information on LATTE can be found at this web site: https://github.com/lanl/LATTE. A brief technical description is given with the *fix latte* command.

Authors: Christian Negre (LANL) and Steve Plimpton (Sandia). LATTE itself is developed at Los Alamos National Laboratory by Marc Cawkwell, Anders Niklasson, and Christian Negre.

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/LATTE: filenames -> commands
- src/LATTE/README
- lib/latte/README
- *fix latte*
- examples/latte
- LAMMPS-LATTE tutorial

6.3.14 MANYBODY package

Contents:

A variety of many-body and bond-order potentials. These include (AI)REBO, BOP, EAM, EIM, Stillinger-Weber, and Tersoff potentials.

Supporting info:

- src/MANYBODY: filenames -> commands
- *Pair style* page
- examples/comb
- examples/eim
- examples/nb3d
- examples/shear
- examples/streitz
- examples/vashishta
- bench/in.eam

6.3.15 MC package

Contents:

Several fixes and a pair style that have Monte Carlo (MC) or MC-like attributes. These include fixes for creating, breaking, and swapping bonds, for performing atomic swaps, and performing grand-canonical MC (GCMC) in conjunction with dynamics.

Supporting info:

- src/MC: filenames -> commands
- *fix atom/swap*
- *fix bond/break*
- *fix bond/create*
- *fix bond/swap*
- *fix gcmc*
- *pair_style dsmc*
- http://lammps.sandia.gov/movies.html#gcmc

6.3.16 MESSAGE package

Contents:

Commands to use LAMMPS as either a client or server and couple it to another application.

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/MESSAGE: filenames -> commands
- lib/message/README
- *message*
- *fix client/md*
- *server md*
- *server mc*
- examples/message

6.3.17 MISC package

Contents:

A variety of compute, fix, pair, dump styles with specialized capabilities that don't align with other packages. Do a directory listing, "ls src/MISC", to see the list of commands.

Note: the MISC package contains styles that require using the -restrict flag, when compiling with Intel compilers.

Supporting info:

- src/MISC: filenames -> commands
- *compute ti*
- *fix evaporate*
- *fix orient/fcc*
- *fix ttm*
- *fix thermal/conductivity*
- *fix viscosity*
- examples/KAPPA
- examples/VISCOSITY
- http://lammps.sandia.gov/pictures.html#ttm
- http://lammps.sandia.gov/movies.html#evaporation

6.3.18 MOLECULE package

Contents:

A large number of atom, pair, bond, angle, dihedral, improper styles that are used to model molecular systems with fixed covalent bonds. The pair styles include the Dreiding (hydrogen-bonding) and CHARMM force fields, and a TIP4P water model.

Supporting info:

- src/MOLECULE: filenames -> commands
- *atom_style*
- *bond_style*
- *angle_style*
- *dihedral_style*
- *improper_style*
- *pair_style hbond/dreiding/lj*
- *pair_style lj/charmm/coul/charmm*
- *Howto bioFF*
- examples/cmap

- examples/dreiding
- examples/micelle,
- examples/peptide
- bench/in.chain
- bench/in.rhodo

6.3.19 MPIIO package

Contents:

Support for parallel output/input of dump and restart files via the MPIIO library. It adds *dump styles* with a "mpiio" in their style name. Restart files with an ".mpiio" suffix are also written and read in parallel.

Supporting info:

- src/MPIIO: filenames -> commands
- *dump*
- *restart*
- *write_restart*
- *read_restart*

6.3.20 MSCG package

Contents:

A *fix mscg* command which can parameterize a Multi-Scale Coarse-Graining (MSCG) model using the open-source MS-CG library.

To use this package you must have the MS-CG library available on your system.

Authors: The fix was written by Lauren Abbott (Sandia). The MS-CG library was developed by Jacob Wagner in Greg Voth's group at the University of Chicago.

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/MSCG: filenames -> commands
- src/MSCG/README
- lib/mscg/README
- examples/mscg

6.3.21 OPT package

Contents:

A handful of pair styles which are optimized for improved CPU performance on single or multiple cores. These include EAM, LJ, CHARMM, and Morse potentials. The styles have an "opt" suffix in their style name. The *Speed opt* doc page gives details of how to build and use this package. Its styles can be invoked at run time via the "-sf opt" or "-suffix opt" *command-line switches*. See also the *KOKKOS*, *USER-INTEL*, and *USER-OMP* packages, which have styles optimized for CPU performance.

Authors: James Fischer (High Performance Technologies), David Richie, and Vincent Natoli (Stone Ridge Technolgy).

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/OPT: filenames -> commands
- *Speed packages*
- *Speed opt*
- *Section 2.6 -sf opt*
- Search the *pair style* page for styles followed by (t)
- Benchmarks page of web site

6.3.22 PERI package

Contents:

An atom style, several pair styles which implement different Peridynamics materials models, and several computes which calculate diagnostics. Peridynamics is a particle-based meshless continuum model.

Authors: The original package was created by Mike Parks (Sandia). Additional Peridynamics models were added by Rezwanur Rahman and John Foster (UTSA).

Supporting info:

- src/PERI: filenames -> commands
- doc/PDF/PDLammps_overview.pdf
- doc/PDF/PDLammps_EPS.pdf
- doc/PDF/PDLammps_VES.pdf
- *atom_style peri*
- *pair_style peri/**
- *compute damage/atom*
- *compute plasticity/atom*
- examples/peri
- http://lammps.sandia.gov/movies.html#peri

6.3.23 POEMS package

Contents:

A fix that wraps the Parallelizable Open source Efficient Multibody Software (POEMS) library, which is able to simulate the dynamics of articulated body systems. These are systems with multiple rigid bodies (collections of particles) whose motion is coupled by connections at hinge points.

Author: Rudra Mukherjee (JPL) while at RPI.

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/POEMS: filenames -> commands
- src/POEMS/README
- lib/poems/README
- *fix poems*
- examples/rigid

6.3.24 PYTHON package

Contents:

A *python* command which allow you to execute Python code from a LAMMPS input script. The code can be in a separate file or embedded in the input script itself. See the *Python call* doc page for an overview of using Python from LAMMPS in this manner and all the *Python* doc pages for other ways to use LAMMPS and Python together.

Note: Building with the PYTHON package assumes you have a Python shared library available on your system, which needs to be a Python 2 version, 2.6 or later. Python 3 is not yet supported. See the lib/python/README for more details.

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/PYTHON: filenames -> commands
- *Python call*
- lib/python/README
- examples/python

6.3.25 QEQ package

Contents:

Several fixes for performing charge equilibration (QEq) via different algorithms. These can be used with pair styles that perform QEq as part of their formulation.

Supporting info:

- src/QEQ: filenames -> commands
- *fix qeq/**
- examples/qeq
- examples/streitz

6.3.26 REPLICA package

Contents:

A collection of multi-replica methods which can be used when running multiple LAMMPS simulations (replicas). See the *Howto replica* doc page for an overview of how to run multi-replica simulations in LAMMPS. Methods in the package include nudged elastic band (NEB), parallel replica dynamics (PRD), temperature accelerated dynamics (TAD), parallel tempering, and a verlet/split algorithm for performing long-range Coulombics on one set of processors, and the remainder of the force field calculation on another set.

Supporting info:

- src/REPLICA: filenames -> commands
- *Howto replica*
- *neb*
- *prd*
- *tad*
- *temper*,
- *run_style verlet/split*
- examples/neb
- examples/prd
- examples/tad

6.3.27 RIGID package

Contents:

Fixes which enforce rigid constraints on collections of atoms or particles. This includes SHAKE and RATTLE, as well as various rigid-body integrators for a few large bodies or many small bodies. Also several computes which calculate properties of rigid bodies.

Supporting info:

- src/RIGID: filenames -> commands
- *compute erotate/rigid*
- *fix shake*
- *fix rattle*
- *fix rigid/**
- examples/ASPHERE
- examples/rigid
- bench/in.rhodo
- http://lammps.sandia.gov/movies.html#box
- http://lammps.sandia.gov/movies.html#star

6.3.28 SHOCK package

Contents:

Fixes for running impact simulations where a shock-wave passes through a material.

Supporting info:

- src/SHOCK: filenames -> commands
- *fix append/atoms*
- *fix msst*
- *fix nphug*
- *fix wall/piston*
- examples/hugoniostat
- examples/msst

6.3.29 SNAP package

Contents:

A pair style for the spectral neighbor analysis potential (SNAP). SNAP is methodology for deriving a highly accurate classical potential fit to a large archive of quantum mechanical (DFT) data. Also several computes which analyze attributes of the potential.

Author: Aidan Thompson (Sandia).

Supporting info:

- src/SNAP: filenames -> commands
- *pair_style snap*
- *compute sna/atom*
- *compute snad/atom*
- *compute snav/atom*
- examples/snap

6.3.30 SPIN package

Contents:

Model atomic magnetic spins classically, coupled to atoms moving in the usual manner via MD. Various pair, fix, and compute styles.

Author: Julien Tranchida (Sandia).

Supporting info:

- src/SPIN: filenames -> commands
- *Howto spins*
- *pair_style spin/dipole/cut*
- *pair_style spin/dipole/long*
- *pair_style spin/dmi*
- *pair_style spin/exchange*
- *pair_style spin/magelec*
- *pair_style spin/neel*
- *fix nve/spin*
- *fix precession/spin*
- *compute spin*
- *neb/spin*
- examples/SPIN

6.3.31 SRD package

Contents:

A pair of fixes which implement the Stochastic Rotation Dynamics (SRD) method for coarse-graining of a solvent, typically around large colloidal particles.

Supporting info:

- src/SRD: filenames -> commands
- *fix srd*
- *fix wall/srd*
- examples/srd
- examples/ASPHERE
- http://lammps.sandia.gov/movies.html#tri
- http://lammps.sandia.gov/movies.html#line
- http://lammps.sandia.gov/movies.html#poly

6.3.32 VORONOI package

Contents:

A compute command which calculates the Voronoi tesselation of a collection of atoms by wrapping the Voro++ library. This can be used to calculate the local volume or each atoms or its near neighbors.

To use this package you must have the Voro++ library available on your system.

Author: Daniel Schwen (INL) while at LANL. The open-source Voro++ library was written by Chris Rycroft (Harvard U) while at UC Berkeley and LBNL.

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/VORONOI: filenames -> commands
- src/VORONOI/README
- lib/voronoi/README
- *compute voronoi/atom*
- examples/voronoi

6.3.33 USER-ADIOS package

Contents:

ADIOS is a high-performance I/O library. This package implements the *dump atom/adios*, *dump custom/adios* and *read_dump … format adios* commands to write and read data using the ADIOS library.

Authors: Norbert Podhorszki (ORNL) from the ADIOS developer team.

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/USER-ADIOS: filenames -> commands
- src/USER-ADIOS/README
- examples/USER/adios
- https://github.com/ornladios/ADIOS2
- *dump atom/adios*
- *dump custom/adios*
- *read_dump*

6.3.34 USER-ATC package

Contents:

ATC stands for atoms-to-continuum. This package implements a *fix atc* command to either couple molecular dynamics with continuum finite element equations or perform on-the-fly conversion of atomic information to continuum fields.

Authors: Reese Jones, Jeremy Templeton, Jon Zimmerman (Sandia).

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/USER-ATC: filenames -> commands
- src/USER-ATC/README
- *fix atc*
- examples/USER/atc
- http://lammps.sandia.gov/pictures.html#atc

6.3.35 USER-AWPMD package

Contents:

AWPMD stands for Antisymmetrized Wave Packet Molecular Dynamics. This package implements an atom, pair, and fix style which allows electrons to be treated as explicit particles in a classical molecular dynamics model.

Author: Ilya Valuev (JIHT, Russia).

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/USER-AWPMD: filenames -> commands
- src/USER-AWPMD/README
- *pair_style awpmd/cut*
- examples/USER/awpmd

6.3.36 USER-BOCS package

Contents:

This package provides *fix bocs*, a modified version of *fix npt* which includes the pressure correction to the barostat as outlined in:

N. J. H. Dunn and W. G. Noid, "Bottom-up coarse-grained models that accurately describe the structure, pressure, and compressibility of molecular liquids," J. Chem. Phys. 143, 243148 (2015).

Authors: Nicholas J. H. Dunn and Michael R. DeLyser (The Pennsylvania State University)

Supporting info:

The USER-BOCS user package for LAMMPS is part of the BOCS software package: https://github.com/noid-group/BOCS

See the following reference for information about the entire package:

Dunn, NJH; Lebold, KM; DeLyser, MR; Rudzinski, JF; Noid, WG. "BOCS: Bottom-Up Open-Source Coarse-Graining Software." J. Phys. Chem. B. 122, 13, 3363-3377 (2018).

Example inputs are in the examples/USER/bocs folder.

6.3.37 USER-CGDNA package

Contents:

Several pair styles, bond styles, and integration fixes for coarse-grained modelling of single- and double-stranded DNA and RNA based on the oxDNA and oxRNA model of Doye, Louis and Ouldridge. The package includes Langevin-type rigid-body integrators with improved stability.

Author: Oliver Henrich (University of Strathclyde, Glasgow).

Supporting info:

- src/USER-CGDNA: filenames -> commands
- /src/USER-CGDNA/README
- *pair_style oxdna/**
- *pair_style oxdna2/**
- *pair_style oxrna2/**
- *bond_style oxdna/**
- *bond_style oxdna2/**
- *bond_style oxrna2/**
- *fix nve/dotc/langevin*

6.3.38 USER-CGSDK package

Contents:

Several pair styles and an angle style which implement the coarse-grained SDK model of Shinoda, DeVane, and Klein which enables simulation of ionic liquids, electrolytes, lipids and charged amino acids.

Author: Axel Kohlmeyer (Temple U).

Supporting info:

- src/USER-CGSDK: filenames -> commands
- src/USER-CGSDK/README
- *pair_style lj/sdk/**
- *angle_style sdk*
- examples/USER/cgsdk
- http://lammps.sandia.gov/pictures.html#cg

6.3.39 USER-COLVARS package

Contents:

COLVARS stands for collective variables, which can be used to implement various enhanced sampling methods, including Adaptive Biasing Force, Metadynamics, Steered MD, Umbrella Sampling and Restraints. A *fix colvars* command is implemented which wraps a COLVARS library, which implements these methods. simulations.

Authors: The COLVARS library is written and maintained by Giacomo Fiorin (ICMS, Temple University, Philadelphia, PA, USA) and Jerome Henin (LISM, CNRS, Marseille, France), originally for the NAMD MD code, but with portability in mind. Axel Kohlmeyer (Temple U) provided the interface to LAMMPS.

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/USER-COLVARS: filenames -> commands

- doc/PDF/colvars-refman-lammps.pdf
- src/USER-COLVARS/README
- lib/colvars/README
- *fix colvars*
- examples/USER/colvars

6.3.40 USER-PLUMED package

Contents:

The fix plumed command allows you to use the PLUMED free energy plugin for molecular dynamics to analyze and bias your LAMMPS trajectory on the fly. The PLUMED library is called from within the LAMMPS input script by using the *fix plumed* command.

Authors: The *PLUMED library* is written and maintained by Massimilliano Bonomi, Giovanni Bussi, Carlo Camiloni and Gareth Tribello.

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/USER-PLUMED/README
- lib/plumed/README
- *fix plumed*
- examples/USER/plumed

6.3.41 USER-DIFFRACTION package

Contents:

Two computes and a fix for calculating x-ray and electron diffraction intensities based on kinematic diffraction theory.

Author: Shawn Coleman while at the U Arkansas.

Supporting info:

- src/USER-DIFFRACTION: filenames -> commands
- *compute saed*
- *compute xrd*
- *fix saed/vtk*
- examples/USER/diffraction

6.3.42 USER-DPD package

Contents:

DPD stands for dissipative particle dynamics. This package implements coarse-grained DPD-based models for energetic, reactive molecular crystalline materials. It includes many pair styles specific to these systems, including for reactive DPD, where each particle has internal state for multiple species and a coupled set of chemical reaction ODEs are integrated each timestep. Highly accurate time integrators for isothermal, isoenergetic, isobaric and isenthalpic conditions are included. These enable long timesteps via the Shardlow splitting algorithm.

Authors: Jim Larentzos (ARL), Tim Mattox (Engility Corp), and John Brennan (ARL).

Supporting info:

- src/USER-DPD: filenames -> commands
- /src/USER-DPD/README
- *compute dpd*
- *compute dpd/atom*
- *fix eos/cv*
- *fix eos/table*
- *fix eos/table/rx*
- *fix shardlow*
- *fix rx*
- *pair_style table/rx*
- *pair_style dpd/fdt*
- *pair_style dpd/fdt/energy*
- *pair_style exp6/rx*
- *pair_style multi/lucy*
- *pair_style multi/lucy/rx*
- examples/USER/dpd

6.3.43 USER-DRUDE package

Contents:

Fixes, pair styles, and a compute to simulate thermalized Drude oscillators as a model of polarization. See the *Howto drude* and *Howto drude2* doc pages for an overview of how to use the package. There are auxiliary tools for using this package in tools/drude.

Authors: Alain Dequidt (U Blaise Pascal Clermont-Ferrand), Julien Devemy (CNRS), and Agilio Padua (U Blaise Pascal).

Supporting info:

- src/USER-DRUDE: filenames -> commands
- *Howto drude*
- *Howto drude2*

- *Howto polarizable*
- src/USER-DRUDE/README
- *fix drude*
- *fix drude/transform/**
- *compute temp/drude*
- *pair_style thole*
- *pair_style lj/cut/thole/long*
- examples/USER/drude
- tools/drude

6.3.44 USER-EFF package

Contents:

EFF stands for electron force field which allows a classical MD code to model electrons as particles of variable radius. This package contains atom, pair, fix and compute styles which implement the eFF as described in A. Jaramillo-Botero, J. Su, Q. An, and W.A. Goddard III, JCC, 2010. The eFF potential was first introduced by Su and Goddard, in 2007. There are auxiliary tools for using this package in tools/eff; see its README file.

Author: Andres Jaramillo-Botero (CalTech).

Supporting info:

- src/USER-EFF: filenames -> commands
- src/USER-EFF/README
- *atom_style electron*
- *fix nve/eff*
- *fix nvt/eff*
- *fix npt/eff*
- *fix langevin/eff*
- *compute temp/eff*
- *pair_style eff/cut*
- *pair_style eff/inline*
- examples/USER/eff
- tools/eff/README
- tools/eff
- http://lammps.sandia.gov/movies.html#eff

6.3.45 USER-FEP package

Contents:

FEP stands for free energy perturbation. This package provides methods for performing FEP simulations by using a *fix adapt/fep* command with soft-core pair potentials, which have a "soft" in their style name. There are auxiliary tools for using this package in tools/fep; see its README file.

Author: Agilio Padua (Universite Blaise Pascal Clermont-Ferrand)

Supporting info:

- src/USER-FEP: filenames -> commands
- src/USER-FEP/README
- *fix adapt/fep*
- *compute fep*
- *pair_style */soft*
- examples/USER/fep
- tools/fep/README
- tools/fep

6.3.46 USER-H5MD package

Contents:

H5MD stands for HDF5 for MD. HDF5 is a portable, binary, self-describing file format, used by many scientific simulations. H5MD is a format for molecular simulations, built on top of HDF5. This package implements a *dump h5md* command to output LAMMPS snapshots in this format.

To use this package you must have the HDF5 library available on your system.

Author: Pierre de Buyl (KU Leuven) created both the package and the H5MD format.

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/USER-H5MD: filenames -> commands
- src/USER-H5MD/README
- lib/h5md/README
- *dump h5md*

6.3.47 USER-INTEL package

Contents:

Dozens of pair, fix, bond, angle, dihedral, improper, and kspace styles which are optimized for Intel CPUs and KNLs (Knights Landing). All of them have an "intel" in their style name. The *Speed intel* doc page gives details of what hardware and compilers are required on your system, and how to build and use this package. Its styles can be invoked at run time via the "-sf intel" or "-suffix intel" *command-line switches*. Also see the *KOKKOS*, *OPT*, and *USER-OMP* packages, which have styles optimized for CPUs and KNLs.

You need to have an Intel compiler, version 14 or higher to take full advantage of this package. While compilation with GNU compilers is supported, performance will be sub-optimal.

Note: the USER-INTEL package contains styles that require using the -restrict flag, when compiling with Intel compilers.

Author: Mike Brown (Intel).

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/USER-INTEL: filenames -> commands
- src/USER-INTEL/README
- *Speed packages*
- *Speed intel*
- *Section 2.6 -sf intel*
- *Section 2.6 -pk intel*
- *package intel*
- Search the *commands* pages (*fix*, *compute*, *pair*, *bond, angle, dihedral, improper*, *kspace*) for styles followed by (i)
- src/USER-INTEL/TEST
- Benchmarks page of web site

6.3.48 USER-LB package

Contents:

Fixes which implement a background Lattice-Boltzmann (LB) fluid, which can be used to model MD particles influenced by hydrodynamic forces.

Authors: Frances Mackay and Colin Denniston (University of Western Ontario).

Supporting info:

- src/USER-LB: filenames -> commands
- src/USER-LB/README
- *fix lb/fluid*

- *fix lb/momentum*
- *fix lb/viscous*
- examples/USER/lb

6.3.49 USER-MGPT package

Contents:

A pair style which provides a fast implementation of the quantum-based MGPT multi-ion potentials. The MGPT or model GPT method derives from first-principles DFT-based generalized pseudopotential theory (GPT) through a series of systematic approximations valid for mid-period transition metals with nearly half-filled d bands. The MGPT method was originally developed by John Moriarty at LLNL. The pair style in this package calculates forces and energies using an optimized matrix-MGPT algorithm due to Tomas Oppelstrup at LLNL.

Authors: Tomas Oppelstrup and John Moriarty (LLNL).

Supporting info:

- src/USER-MGPT: filenames -> commands
- src/USER-MGPT/README
- *pair_style mgpt*
- examples/USER/mgpt

6.3.50 USER-MISC package

Contents:

A potpourri of (mostly) unrelated features contributed to LAMMPS by users. Each feature is a single fix, compute, pair, bond, angle, dihedral, improper, or command style.

Authors: The author for each style in the package is listed in the src/USER-MISC/README file.

Supporting info:

- src/USER-MISC: filenames -> commands
- src/USER-MISC/README
- one doc page per individual command listed in src/USER-MISC/README
- examples/USER/misc

6.3.51 USER-MANIFOLD package

Contents:

Several fixes and a "manifold" class which enable simulations of particles constrained to a manifold (a 2D surface within the 3D simulation box). This is done by applying the RATTLE constraint algorithm to formulate single-particle constraint functions g(xi,yi,zi) = 0 and their derivative (i.e. the normal of the manifold) n = grad(g).

Author: Stefan Paquay (until 2017: Eindhoven University of Technology (TU/e), The Netherlands; since 2017: Brandeis University, Waltham, MA, USA)

Supporting info:

- src/USER-MANIFOLD: filenames -> commands
- src/USER-MANIFOLD/README
- *Howto manifold*
- *fix manifoldforce*
- *fix nve/manifold/rattle*
- *fix nvt/manifold/rattle*
- examples/USER/manifold
- http://lammps.sandia.gov/movies.html#manifold

6.3.52 USER-MEAMC package

Contents:

A pair style for the modified embedded atom (MEAM) potential translated from the Fortran version in the (obsolete) "MEAM" package to plain C++. The USER-MEAMC fully replaces the MEAM package, which has been removed from LAMMPS after the 12 December 2018 version.

Author: Sebastian Huetter, (Otto-von-Guericke University Magdeburg) based on the Fortran version of Greg Wagner (Northwestern U) while at Sandia.

Supporting info:

- src/USER-MEAMC: filenames -> commands
- src/USER-MEAMC/README
- *pair_style meam/c*
- examples/meamc

6.3.53 USER-MESO package

Contents:

Several extensions of the dissipative particle dynamics (DPD) method. Specifically, energy-conserving DPD (eDPD) that can model non-isothermal processes, many-body DPD (mDPD) for simulating vapor-liquid coexistence, and transport DPD (tDPD) for modeling advection-diffusion-reaction systems. The equations of motion of these DPD extensions are integrated through a modified velocity-Verlet (MVV) algorithm.

Author: Zhen Li (Division of Applied Mathematics, Brown University)

Supporting info:

- src/USER-MESO: filenames -> commands
- src/USER-MESO/README
- *atom_style edpd*
- *pair_style edpd*
- *pair_style mdpd*
- *pair_style tdpd*
- *fix mvv/dpd*
- examples/USER/meso
- http://lammps.sandia.gov/movies.html#mesodpd

6.3.54 USER-MOFFF package

Contents:

Pair, angle and improper styles needed to employ the MOF-FF force field by Schmid and coworkers with LAMMPS. MOF-FF is a first principles derived force field with the primary aim to simulate MOFs and related porous framework materials, using spherical Gaussian charges. It is described in S. Bureekaew et al., Phys. Stat. Sol. B 2013, 250, 1128-1141. For the usage of MOF-FF see the example in the example directory as well as the MOF+ website.

Author: Hendrik Heenen (Technical U of Munich), Rochus Schmid (Ruhr-University Bochum).

Supporting info:

- src/USER-MOFFF: filenames -> commands
- src/USER-MOFFF/README
- *pair_style buck6d/coul/gauss*
- *angle_style class2*
- *angle_style cosine/buck6d*
- *improper_style inversion/harmonic*
- examples/USER/mofff

6.3.55 USER-MOLFILE package

Contents:

A *dump molfile* command which uses molfile plugins that are bundled with the VMD molecular visualization and analysis program, to enable LAMMPS to dump snapshots in formats compatible with various molecular simulation tools.

To use this package you must have the desired VMD plugins available on your system.

Note that this package only provides the interface code, not the plugins themselves, which will be accessed when requesting a specific plugin via the *dump molfile* command. Plugins can be obtained from a VMD installation which has to match the platform that you are using to compile LAMMPS for. By adding plugins to VMD, support for new file formats can be added to LAMMPS (or VMD or other programs that use them) without having to re-compile the application itself. More information about the VMD molfile plugins can be found at http://www.ks.uiuc.edu/Research/vmd/plugins/molfile.

Author: Axel Kohlmeyer (Temple U).

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/USER-MOLFILE: filenames -> commands
- src/USER-MOLFILE/README
- lib/molfile/README
- *dump molfile*

6.3.56 USER-NETCDF package

Contents:

Dump styles for writing NetCDF formatted dump files. NetCDF is a portable, binary, self-describing file format developed on top of HDF5. The file contents follow the AMBER NetCDF trajectory conventions (http://ambermd.org/netcdf/nctraj.xhtml), but include extensions.

To use this package you must have the NetCDF library available on your system.

Note that NetCDF files can be directly visualized with the following tools:

- Ovito (Ovito supports the AMBER convention and the extensions mentioned above)
- VMD
- AtomEye (the libAtoms version of AtomEye contains a NetCDF reader not present in the standard distribution)

Author: Lars Pastewka (Karlsruhe Institute of Technology).

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/USER-NETCDF: filenames -> commands
- src/USER-NETCDF/README

- lib/netcdf/README
- *dump netcdf*

6.3.57 USER-OMP package

Contents:

Hundreds of pair, fix, compute, bond, angle, dihedral, improper, and kspace styles which are altered to enable threading on many-core CPUs via OpenMP directives. All of them have an "omp" in their style name. The *Speed omp* doc page gives details of what hardware and compilers are required on your system, and how to build and use this package. Its styles can be invoked at run time via the "-sf omp" or "-suffix omp" *command-line switches*. Also see the *KOKKOS*, *OPT*, and *USER-INTEL* packages, which have styles optimized for CPUs.

Author: Axel Kohlmeyer (Temple U).

Note: To enable multi-threading support the compile flag "-fopenmp" and the link flag "-fopenmp" (for GNU compilers, you have to look up the equivalent flags for other compilers) must be used to build LAMMPS. When using Intel compilers, also the "-restrict" flag is required. The USER-OMP package can be compiled without enabling OpenMP; then all code will be compiled as serial and the only improvement over the regular styles are some data access optimization. These flags should be added to the CCFLAGS and LINKFLAGS lines of your Makefile.machine. See src/MAKE/OPTIONS/Makefile.omp for an example.

Once you have an appropriate Makefile.machine, you can install/un-install the package and build LAMMPS in the usual manner:

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/USER-OMP: filenames -> commands
- src/USER-OMP/README
- *Speed packages*
- *Speed omp*
- *Section 2.6 -sf omp*
- *Section 2.6 -pk omp*
- *package omp*
- Search the *commands* pages (*fix*, *compute*, *pair*, *bond, angle, dihedral, improper*, *kspace*) for styles followed by (o)
- Benchmarks page of web site

6.3.58 USER-PHONON package

Contents:

A *fix phonon* command that calculates dynamical matrices, which can then be used to compute phonon dispersion relations, directly from molecular dynamics simulations. And a *dynamical_matrix* as well as a *third_order* command to compute the dynamical matrix and third order tensor from finite differences.

Authors: Ling-Ti Kong (Shanghai Jiao Tong University) for "fix phonon" and Charlie Sievers (UC Davis) for "dynamical_matrix" and "third_order"

Supporting info:

- src/USER-PHONON: filenames -> commands
- src/USER-PHONON/README
- *fix phonon*
- *dynamical_matrix*
- *third_order*
- examples/USER/phonon

6.3.59 USER-PTM package

Contents:

A *compute ptm/atom* command that calculates local structure characterization using the Polyhedral Template Matching methodology.

Author: Peter Mahler Larsen (MIT).

Supporting info:

- src/USER-PTM: filenames not starting with ptm_ -> commands
- src/USER-PTM: filenames starting with ptm_ -> supporting code
- src/USER-PTM/LICENSE
- *compute ptm/atom*

6.3.60 USER-QMMM package

Contents:

A *fix qmmm* command which allows LAMMPS to be used as the MM code in a QM/MM simulation. This is currently only available in combination with the Quantum ESPRESSO package.

To use this package you must have Quantum ESPRESSO (QE) available on your system and include its coupling library in the compilation and then compile LAMMPS as a library. For QM/MM calculations you then build a custom binary with MPI support, that sets up 3 partitions with MPI sub-communicators (for inter- and intra-partition communication) and then calls the corresponding library interfaces on each partition (2x LAMMPS and 1x QE).

The current implementation supports an ONIOM style mechanical coupling and a multi-pole based electrostatic coupling to the Quantum ESPRESSO plane wave DFT package. The QM/MM interface has been written in a manner that coupling to other QM codes should be possible without changes to LAMMPS itself.

Authors: Axel Kohlmeyer (Temple U). Mariella Ippolito and Carlo Cavazzoni (CINECA, Italy)

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/USER-QMMM: filenames -> commands
- src/USER-QMMM/README
- lib/qmmm/README
- *fix phonon*
- lib/qmmm/example-ec/README
- lib/qmmm/example-mc/README

6.3.61 USER-QTB package

Contents:

Two fixes which provide a self-consistent quantum treatment of vibrational modes in a classical molecular dynamics simulation. By coupling the MD simulation to a colored thermostat, it introduces zero point energy into the system, altering the energy power spectrum and the heat capacity to account for their quantum nature. This is useful when modeling systems at temperatures lower than their classical limits or when temperatures ramp across the classical limits in a simulation.

Author: Yuan Shen (Stanford U).

Supporting info:

- src/USER-QTB: filenames -> commands
- src/USER-QTB/README
- *fix qtb*
- *fix qbmsst*
- examples/USER/qtb

6.3.62 USER-QUIP package

Contents:

A *pair_style quip* command which wraps the QUIP libAtoms library, which includes a variety of interatomic potentials, including Gaussian Approximation Potential (GAP) models developed by the Cambridge University group.

To use this package you must have the QUIP libAtoms library available on your system.

Author: Albert Bartok (Cambridge University)

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/USER-QUIP: filenames -> commands
- src/USER-QUIP/README
- *pair_style quip*
- examples/USER/quip

6.3.63 USER-REAXC package

Contents:

A pair style which implements the ReaxFF potential in C/C++. ReaxFF is a universal reactive force field. See the src/USER-REAXC/README file for more info on differences between the two packages. Also two fixes for monitoring molecules as bonds are created and destroyed.

Author: Hasan Metin Aktulga (MSU) while at Purdue University.

Supporting info:

- src/USER-REAXC: filenames -> commands
- src/USER-REAXC/README
- *pair_style reax/c*
- *fix reax/c/bonds*
- *fix reax/c/species*
- examples/reax

6.3.64 USER-SCAFACOS package

Contents:

A KSpace style which wraps the ScaFaCoS Coulomb solver library to compute long-range Coulombic interactions.

To use this package you must have the ScaFaCoS library available on your system.

Author: Rene Halver (JSC) wrote the scafacos LAMMPS command.

ScaFaCoS itself was developed by a consortium of German research facilities with a BMBF (German Ministry of Science and Education) funded project in 2009-2012. Participants of the consortium were the Universities of Bonn, Chemnitz, Stuttgart, and Wuppertal as well as the Forschungszentrum Juelich.

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/USER-SCAFACOS: filenames -> commands
- src/USER-SCAFACOS/README
- *kspace_style scafacos*
- *kspace_modify*
- examples/USER/scafacos

6.3.65 USER-SDPD package

Contents:

A pair style for smoothed dissipative particle dynamics (SDPD), which is an extension of smoothed particle hydrodynamics (SPH) to mesoscale where thermal fluctuations are important (see the *USER-SPH package*). Also two fixes for moving and rigid body integration of SPH/SDPD particles (particles of atom_style meso).

Author: Morteza Jalalvand (Institute for Advanced Studies in Basic Sciences, Iran).

Supporting info:

- src/USER-SDPD: filenames -> commands
- src/USER-SDPD/README
- *pair_style sdpd/taitwater/isothermal*
- *fix meso/move*
- *fix rigid/meso*
- examples/USER/sdpd

6.3.66 USER-SMD package

Contents:

An atom style, fixes, computes, and several pair styles which implements smoothed Mach dynamics (SMD) for solids, which is a model related to smoothed particle hydrodynamics (SPH) for liquids (see the *USER-SPH package*).

This package solves solids mechanics problems via a state of the art stabilized meshless method with hourglass control. It can specify hydrostatic interactions independently from material strength models, i.e. pressure and deviatoric stresses are separated. It provides many material models (Johnson-Cook, plasticity with hardening, Mie-Grueneisen, Polynomial EOS) and allows new material models to be added. It implements rigid boundary conditions (walls) which can be specified as surface geometries from *.STL files.

Author: Georg Ganzenmuller (Fraunhofer-Institute for High-Speed Dynamics, Ernst Mach Institute, Germany).

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/USER-SMD: filenames -> commands
- src/USER-SMD/README
- doc/PDF/SMD_LAMMPS_userguide.pdf
- examples/USER/smd
- http://lammps.sandia.gov/movies.html#smd

6.3.67 USER-SMTBQ package

Contents:

A pair style which implements a Second Moment Tight Binding model with QEq charge equilibration (SMTBQ) potential for the description of ionocovalent bonds in oxides.

Authors: Nicolas Salles, Emile Maras, Olivier Politano, and Robert Tetot (LAAS-CNRS, France).

Supporting info:

- src/USER-SMTBQ: filenames -> commands
- src/USER-SMTBQ/README
- *pair_style smtbq*
- examples/USER/smtbq

6.3.68 USER-SPH package

Contents:

An atom style, fixes, computes, and several pair styles which implements smoothed particle hydrodynamics (SPH) for liquids. See the related *USER-SMD package* package for smooth Mach dynamics (SMD) for solids.

This package contains ideal gas, Lennard-Jones equation of states, Tait, and full support for complete (i.e. internal-energy dependent) equations of state. It allows for plain or Monaghans XSPH integration of the equations of motion. It has options for density continuity or density summation to propagate the density field. It has *set* command options to set the internal energy and density of particles from the input script and allows the same quantities to be output with thermodynamic output or to dump files via the *compute property/atom* command.

Author: Georg Ganzenmuller (Fraunhofer-Institute for High-Speed Dynamics, Ernst Mach Institute, Germany).

Supporting info:

- src/USER-SPH: filenames -> commands
- src/USER-SPH/README
- doc/PDF/SPH_LAMMPS_userguide.pdf
- examples/USER/sph
- http://lammps.sandia.gov/movies.html#sph

6.3.69 USER-TALLY package

Contents:

Several compute styles that can be called when pairwise interactions are calculated to tally information (forces, heat flux, energy, stress, etc) about individual interactions.

Author: Axel Kohlmeyer (Temple U).

Supporting info:

- src/USER-TALLY: filenames -> commands

- src/USER-TALLY/README
- *compute */tally*
- examples/USER/tally

6.3.70 USER-UEF package

Contents:

A fix style for the integration of the equations of motion under extensional flow with proper boundary conditions, as well as several supporting compute styles and an output option.

Author: David Nicholson (MIT).

Supporting info:

- src/USER-UEF: filenames -> commands
- src/USER-UEF/README
- *fix nvt/uef*
- *fix npt/uef*
- *compute pressure/uef*
- *compute temp/uef*
- *dump cfg/uef*
- examples/uef

6.3.71 USER-VTK package

Contents:

A *dump vtk* command which outputs snapshot info in the VTK format, enabling visualization by Paraview or other visualization packages.

To use this package you must have VTK library available on your system.

Authors: Richard Berger (JKU) and Daniel Queteschiner (DCS Computing).

Install:

This package has *specific installation instructions* on the *Build extras* doc page.

Supporting info:

- src/USER-VTK: filenames -> commands
- src/USER-VTK/README
- lib/vtk/README
- *dump vtk*

6.3.72 USER-YAFF package

Contents:

Some potentials that are also implemented in the Yet Another Force Field (YAFF) code. The expressions and their use are discussed in the following papers

- Vanduyfhuys et al., J. Comput. Chem., 36 (13), 1015-1027 (2015) link
- Vanduyfhuys et al., J. Comput. Chem., 39 (16), 999-1011 (2018) link

which discuss the QuickFF methodology.

Author: Steven Vandenbrande.

Supporting info:

- src/USER-YAFF/README
- *angle_style cross*
- *angle_style mm3*
- *bond_style mm3*
- *improper_style distharm*
- *improper_style sqdistharm*
- *pair_style mm3/switch3/coulgauss/long*
- *pair_style lj/switch3/coulgauss/long*
- examples/USER/yaff

CHAPTER

SEVEN

ACCELERATE PERFORMANCE

This section describes various methods for improving LAMMPS performance for different classes of problems running on different kinds of machines.

There are two thrusts to the discussion that follows. The first is using code options that implement alternate algorithms that can speed-up a simulation. The second is to use one of the several accelerator packages provided with LAMMPS that contain code optimized for certain kinds of hardware, including multi-core CPUs, GPUs, and Intel Xeon Phi co-processors.

The Benchmark page of the LAMMPS web site gives performance results for the various accelerator packages discussed on the *Speed packages* doc page, for several of the standard LAMMPS benchmark problems, as a function of problem size and number of compute nodes, on different hardware platforms.

7.1 Benchmarks

Current LAMMPS performance is discussed on the Benchmarks page of the LAMMPS website where timings and parallel efficiency are listed. The page has several sections, which are briefly described below:

- CPU performance on 5 standard problems, strong and weak scaling
- GPU and Xeon Phi performance on same and related problems
- Comparison of cost of interatomic potentials
- Performance of huge, billion-atom problems

The 5 standard problems are as follow:

1. LJ = atomic fluid, Lennard-Jones potential with 2.5 sigma cutoff (55 neighbors per atom), NVE integration
2. Chain = bead-spring polymer melt of 100-mer chains, FENE bonds and LJ pairwise interactions with a 2^(1/6) sigma cutoff (5 neighbors per atom), NVE integration
3. EAM = metallic solid, Cu EAM potential with 4.95 Angstrom cutoff (45 neighbors per atom), NVE integration
4. Chute = granular chute flow, frictional history potential with 1.1 sigma cutoff (7 neighbors per atom), NVE integration
5. Rhodo = rhodopsin protein in solvated lipid bilayer, CHARMM force field with a 10 Angstrom LJ cutoff (440 neighbors per atom), particle-particle particle-mesh (PPPM) for long-range Coulombics, NPT integration

Input files for these 5 problems are provided in the bench directory of the LAMMPS distribution. Each has 32,000 atoms and runs for 100 timesteps. The size of the problem (number of atoms) can be varied using command-line switches as described in the bench/README file. This is an easy way to test performance and either strong or weak scalability on your machine.

The bench directory includes a few log.* files that show performance of these 5 problems on 1 or 4 cores of Linux desktop. The bench/FERMI and bench/KEPLER directories have input files and scripts and instructions for running the same (or similar) problems using OpenMP or GPU or Xeon Phi acceleration options. See the README files in those directories and the *Speed packages* doc pages for instructions on how to build LAMMPS and run on that kind of hardware.

The bench/POTENTIALS directory has input files which correspond to the table of results on the Potentials section of the Benchmarks web page. So you can also run those test problems on your machine.

The billion-atom section of the Benchmarks web page has performance data for very large benchmark runs of simple Lennard-Jones (LJ) models, which use the bench/in.lj input script.

For all the benchmarks, a useful metric is the CPU cost per atom per timestep. Since performance scales roughly linearly with problem size and timesteps for all LAMMPS models (i.e. interatomic or coarse-grained potentials), the run time of any problem using the same model (atom style, force field, cutoff, etc) can then be estimated.

Performance on a parallel machine can also be predicted from one-core or one-node timings if the parallel efficiency can be estimated. The communication bandwidth and latency of a particular parallel machine affects the efficiency. On most machines LAMMPS will give a parallel efficiency on these benchmarks above 50% so long as the number of atoms/core is a few 100 or greater, and closer to 100% for large numbers of atoms/core. This is for all-MPI mode with one MPI task per core. For nodes with accelerator options or hardware (OpenMP, GPU, Phi), you should first measure single node performance. Then you can estimate parallel performance for multi-node runs using the same logic as for all-MPI mode, except that now you will typically need many more atoms/node to achieve good scalability.

7.2 Measuring performance

Before trying to make your simulation run faster, you should understand how it currently performs and where the bottlenecks are.

The best way to do this is run the your system (actual number of atoms) for a modest number of timesteps (say 100 steps) on several different processor counts, including a single processor if possible. Do this for an equilibrium version of your system, so that the 100-step timings are representative of a much longer run. There is typically no need to run for 1000s of timesteps to get accurate timings; you can simply extrapolate from short runs.

For the set of runs, look at the timing data printed to the screen and log file at the end of each LAMMPS run. The *Run_output* doc page gives an overview.

Running on one (or a few processors) should give a good estimate of the serial performance and what portions of the timestep are taking the most time. Running the same problem on a few different processor counts should give an estimate of parallel scalability. I.e. if the simulation runs 16x faster on 16 processors, its 100% parallel efficient; if it runs 8x faster on 16 processors, it's 50% efficient.

The most important data to look at in the timing info is the timing breakdown and relative percentages. For example, trying different options for speeding up the long-range solvers will have little impact if they only consume 10% of the run time. If the pairwise time is dominating, you may want to look at GPU or OMP versions of the pair style, as discussed below. Comparing how the percentages change as you increase the processor count gives you a sense of how different operations within the timestep are scaling. Note that if you are running with a Kspace solver, there is additional output on the breakdown of the Kspace time. For PPPM, this includes the fraction spent on FFTs, which can be communication intensive.

Another important detail in the timing info are the histograms of atoms counts and neighbor counts. If these vary widely across processors, you have a load-imbalance issue. This often results in inaccurate relative timing data, because processors have to wait when communication occurs for other processors to catch up. Thus the reported times for "Communication" or "Other" may be higher than they really are, due to load-imbalance. If this is an issue, you can uncomment the MPI_Barrier() lines in src/timer.cpp, and re-compile LAMMPS, to obtain synchronized timings.

7.3 General tips

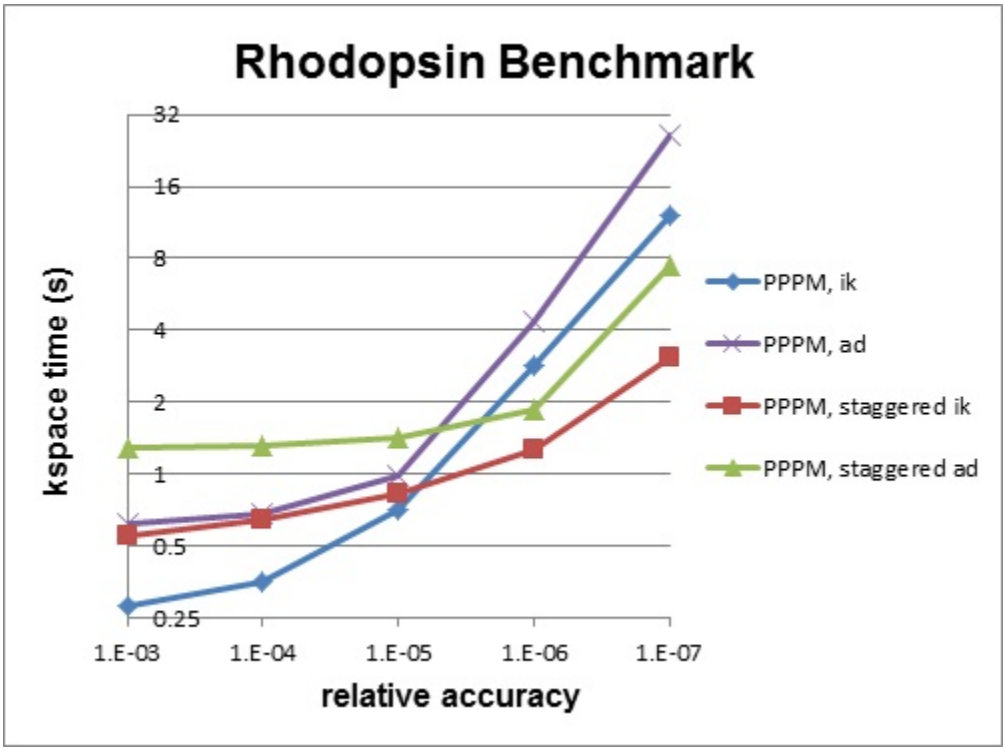
Note: this page is still a work in progress

Here is a list of general ideas for improving simulation performance. Most of them are only applicable to certain models and certain bottlenecks in the current performance, so let the timing data you generate be your guide. It is hard, if not impossible, to predict how much difference these options will make, since it is a function of problem size, number of processors used, and your machine. There is no substitute for identifying performance bottlenecks, and trying out various options.

- rRESPA
- Two-FFT PPPM
- Staggered PPPM
- single vs double PPPM
- partial charge PPPM
- verlet/split run style
- processor command for proc layout and numa layout
- load-balancing: balance and fix balance

Two-FFT PPPM, also called *analytic differentiation* or *ad* PPPM, uses 2 FFTs instead of the 4 FFTs used by the default *ik differentiation* PPPM. However, 2-FFT PPPM also requires a slightly larger mesh size to achieve the same accuracy as 4-FFT PPPM. For problems where the FFT cost is the performance bottleneck (typically large problems running on many processors), 2-FFT PPPM may be faster than 4-FFT PPPM.

Staggered PPPM performs calculations using two different meshes, one shifted slightly with respect to the other. This can reduce force aliasing errors and increase the accuracy of the method, but also doubles the amount of work required. For high relative accuracy, using staggered PPPM allows one to half the mesh size in each dimension as compared to regular PPPM, which can give around a 4x speedup in the kspace time. However, for low relative accuracy, using staggered PPPM gives little benefit and can be up to 2x slower in the kspace time. For example, the rhodopsin benchmark was run on a single processor, and results for kspace time vs. relative accuracy for the different methods are shown in the figure below. For this system, staggered PPPM (using ik differentiation) becomes useful when using a relative accuracy of slightly greater than 1e-5 and above.



Note: Using staggered PPPM may not give the same increase in accuracy of energy and pressure as it does in forces, so some caution must be used if energy and/or pressure are quantities of interest, such as when using a barostat.

7.4 Accelerator packages

Accelerated versions of various *pair_style*, *fixes*, *computes*, and other commands have been added to LAMMPS, which will typically run faster than the standard non-accelerated versions. Some require appropriate hardware to be present on your system, e.g. GPUs or Intel Xeon Phi co-processors.

All of these commands are in packages provided with LAMMPS. An overview of packages is give on the *Packages* doc pages.

These are the accelerator packages currently in LAMMPS, either as standard or user packages:

GPU Package	for NVIDIA GPUs as well as OpenCL support
USER-INTEL Package	for Intel CPUs and Intel Xeon Phi
KOKKOS Package	for Nvidia GPUs, Intel Xeon Phi, and OpenMP threading
USER-OMP Package	for OpenMP threading and generic CPU optimizations
OPT Package	generic CPU optimizations

7.4.1 GPU package

The GPU package was developed by Mike Brown while at SNL and ORNL and his collaborators, particularly Trung Nguyen (now at Northwestern). It provides GPU versions of many pair styles and for parts of the *kspace_style pppm* for long-range Coulombics. It has the following general features:

- It is designed to exploit common GPU hardware configurations where one or more GPUs are coupled to many cores of one or more multi-core CPUs, e.g. within a node of a parallel machine.
- Atom-based data (e.g. coordinates, forces) are moved back-and-forth between the CPU(s) and GPU every timestep.
- Neighbor lists can be built on the CPU or on the GPU
- The charge assignment and force interpolation portions of PPPM can be run on the GPU. The FFT portion, which requires MPI communication between processors, runs on the CPU.
- Force computations of different style (pair vs. bond/angle/dihedral/improper) can be performed concurrently on the GPU and CPU(s), respectively.
- It allows for GPU computations to be performed in single or double precision, or in mixed-mode precision, where pairwise forces are computed in single precision, but accumulated into double-precision force vectors.
- LAMMPS-specific code is in the GPU package. It makes calls to a generic GPU library in the lib/gpu directory. This library provides NVIDIA support as well as more general OpenCL support, so that the same functionality is supported on a variety of hardware.

Required hardware/software:

To compile and use this package in CUDA mode, you currently need to have an NVIDIA GPU and install the corresponding NVIDIA CUDA toolkit software on your system (this is primarily tested on Linux and completely unsupported on Windows):

- Check if you have an NVIDIA GPU: cat /proc/driver/nvidia/gpus/*/information
- Go to http://www.nvidia.com/object/cuda_get.html
- Install a driver and toolkit appropriate for your system (SDK is not necessary)
- Run lammps/lib/gpu/nvc_get_devices (after building the GPU library, see below) to list supported devices and properties

To compile and use this package in OpenCL mode, you currently need to have the OpenCL headers and the (vendor neutral) OpenCL library installed. In OpenCL mode, the acceleration depends on having an OpenCL Installable Client Driver (ICD) installed. There can be multiple of them for the same or different hardware (GPUs, CPUs, Accelerators) installed at the same time. OpenCL refers to those as 'platforms'. The GPU library will select the **first** suitable platform, but this can be overridden using the device option of the *package* command. run lammps/lib/gpu/ocl_get_devices to get a list of available platforms and devices with a suitable ICD available.

Building LAMMPS with the GPU package:

See the *Build extras* doc page for instructions.

Run with the GPU package from the command line:

The mpirun or mpiexec command sets the total number of MPI tasks used by LAMMPS (one or multiple per compute node) and the number of MPI tasks used per node. E.g. the mpirun command in MPICH does this via its -np and -ppn switches. Ditto for OpenMPI via -np and -npernode.

When using the GPU package, you cannot assign more than one GPU to a single MPI task. However multiple MPI tasks can share the same GPU, and in many cases it will be more efficient to run this way. Likewise it may be more efficient to use less MPI tasks/node than the available # of CPU cores. Assignment of multiple MPI tasks to a GPU

will happen automatically if you create more MPI tasks/node than there are GPUs/mode. E.g. with 8 MPI tasks/node and 2 GPUs, each GPU will be shared by 4 MPI tasks.

Use the "-sf gpu" *command-line switch*, which will automatically append "gpu" to styles that support it. Use the "-pk gpu Ng" *command-line switch* to set Ng = # of GPUs/node to use.

```
lmp_machine -sf gpu -pk gpu 1 -in in.script                         # 1 MPI task uses␣
↪1 GPU
mpirun -np 12 lmp_machine -sf gpu -pk gpu 2 -in in.script           # 12 MPI tasks␣
↪share 2 GPUs on a single 16-core (or whatever) node
mpirun -np 48 -ppn 12 lmp_machine -sf gpu -pk gpu 2 -in in.script   # ditto on 4 16-
↪core nodes
```

Note that if the "-sf gpu" switch is used, it also issues a default *package gpu 1* command, which sets the number of GPUs/node to 1.

Using the "-pk" switch explicitly allows for setting of the number of GPUs/node to use and additional options. Its syntax is the same as same as the "package gpu" command. See the *package* command doc page for details, including the default values used for all its options if it is not specified.

Note that the default for the *package gpu* command is to set the Newton flag to "off" pairwise interactions. It does not affect the setting for bonded interactions (LAMMPS default is "on"). The "off" setting for pairwise interaction is currently required for GPU package pair styles.

Or run with the GPU package by editing an input script:

The discussion above for the mpirun/mpiexec command, MPI tasks/node, and use of multiple MPI tasks/GPU is the same.

Use the *suffix gpu* command, or you can explicitly add an "gpu" suffix to individual styles in your input script, e.g.

```
pair_style lj/cut/gpu 2.5
```

You must also use the *package gpu* command to enable the GPU package, unless the "-sf gpu" or "-pk gpu" *command-line switches* were used. It specifies the number of GPUs/node to use, as well as other options.

Speed-ups to expect:

The performance of a GPU versus a multi-core CPU is a function of your hardware, which pair style is used, the number of atoms/GPU, and the precision used on the GPU (double, single, mixed). Using the GPU package in OpenCL mode on CPUs (which uses vectorization and multithreading) is usually resulting in inferior performance compared to using LAMMPS' native threading and vectorization support in the USER-OMP and USER-INTEL packages.

See the Benchmark page of the LAMMPS web site for performance of the GPU package on various hardware, including the Titan HPC platform at ORNL.

You should also experiment with how many MPI tasks per GPU to use to give the best performance for your problem and machine. This is also a function of the problem size and the pair style being using. Likewise, you should experiment with the precision setting for the GPU library to see if single or mixed precision will give accurate results, since they will typically be faster.

Guidelines for best performance:

- Using multiple MPI tasks per GPU will often give the best performance, as allowed my most multi-core CPU/GPU configurations.
- If the number of particles per MPI task is small (e.g. 100s of particles), it can be more efficient to run with fewer MPI tasks per GPU, even if you do not use all the cores on the compute node.
- The *package gpu* command has several options for tuning performance. Neighbor lists can be built on the GPU or CPU. Force calculations can be dynamically balanced across the CPU cores and GPUs. GPU-specific settings can be made which can be optimized for different hardware. See the *package* command doc page for details.

- As described by the *package gpu* command, GPU accelerated pair styles can perform computations asynchronously with CPU computations. The "Pair" time reported by LAMMPS will be the maximum of the time required to complete the CPU pair style computations and the time required to complete the GPU pair style computations. Any time spent for GPU-enabled pair styles for computations that run simultaneously with *bond*, *angle*, *dihedral*, *improper*, and *long-range* calculations will not be included in the "Pair" time.
- When the *mode* setting for the package gpu command is force/neigh, the time for neighbor list calculations on the GPU will be added into the "Pair" time, not the "Neigh" time. An additional breakdown of the times required for various tasks on the GPU (data copy, neighbor calculations, force computations, etc) are output only with the LAMMPS screen output (not in the log file) at the end of each run. These timings represent total time spent on the GPU for each routine, regardless of asynchronous CPU calculations.
- The output section "GPU Time Info (average)" reports "Max Mem / Proc". This is the maximum memory used at one time on the GPU for data storage by a single MPI process.

Restrictions

None.

7.4.2 USER-INTEL package

The USER-INTEL package is maintained by Mike Brown at Intel Corporation. It provides two methods for accelerating simulations, depending on the hardware you have. The first is acceleration on Intel CPUs by running in single, mixed, or double precision with vectorization. The second is acceleration on Intel Xeon Phi co-processors via offloading neighbor list and non-bonded force calculations to the Phi. The same C++ code is used in both cases. When offloading to a co-processor from a CPU, the same routine is run twice, once on the CPU and once with an offload flag. This allows LAMMPS to run on the CPU cores and co-processor cores simultaneously.

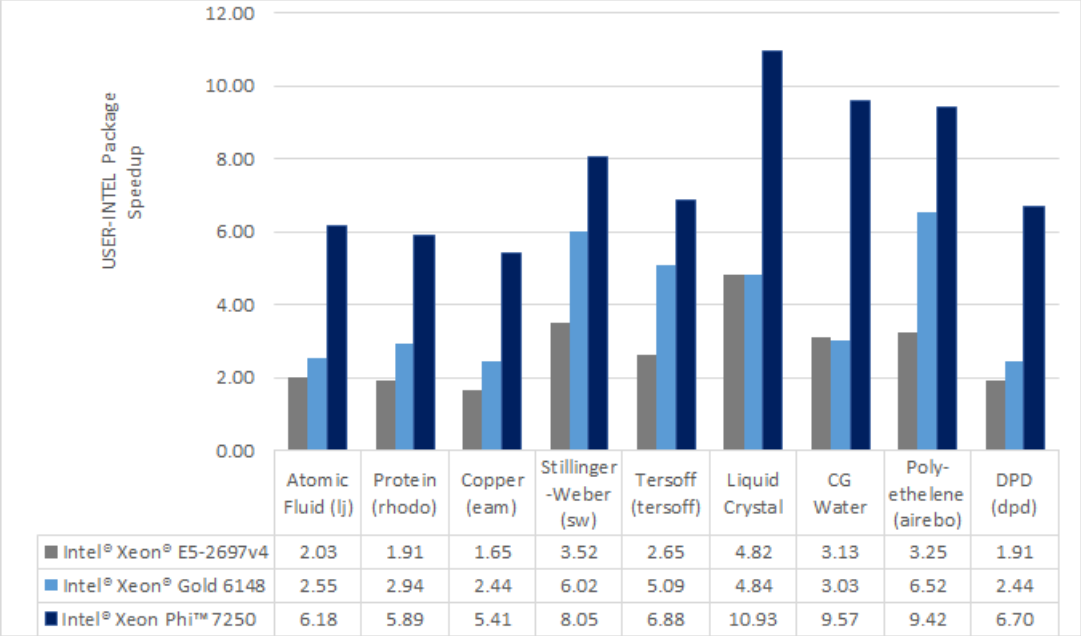
Currently Available USER-INTEL Styles:

- Angle Styles: charmm, harmonic
- Bond Styles: fene, fourier, harmonic
- Dihedral Styles: charmm, fourier, harmonic, opls
- Fixes: nve, npt, nvt, nvt/sllod, nve/asphere
- Improper Styles: cvff, harmonic
- Pair Styles: airebo, airebo/morse, buck/coul/cut, buck/coul/long, buck, dpd, eam, eam/alloy, eam/fs, gayberne, lj/charmm/coul/charmm, lj/charmm/coul/long, lj/cut, lj/cut/coul/long, lj/long/coul/long, rebo, sw, tersoff
- K-Space Styles: pppm, pppm/disp

Warning: None of the styles in the USER-INTEL package currently support computing per-atom stress. If any compute or fix in your input requires it, LAMMPS will abort with an error message.

Speed-ups to expect:

The speedups will depend on your simulation, the hardware, which styles are used, the number of atoms, and the floating-point precision mode. Performance improvements are shown compared to LAMMPS *without using other acceleration packages* as these are under active development (and subject to performance changes). The measurements were performed using the input files available in the src/USER-INTEL/TEST directory with the provided run script. These are scalable in size; the results given are with 512K particles (524K for Liquid Crystal). Most of the simulations are standard LAMMPS benchmarks (indicated by the filename extension in parenthesis) with modifications to the run length and to add a warm-up run (for use with offload benchmarks).



Results are speedups obtained on Intel Xeon E5-2697v4 processors (code-named Broadwell), Intel Xeon Phi 7250 processors (code-named Knights Landing), and Intel Xeon Gold 6148 processors (code-named Skylake) with "June 2017" LAMMPS built with Intel Parallel Studio 2017 update 2. Results are with 1 MPI task per physical core. See *src/USER-INTEL/TEST/README* for the raw simulation rates and instructions to reproduce.

Accuracy and order of operations:

In most molecular dynamics software, parallelization parameters (# of MPI, OpenMP, and vectorization) can change the results due to changing the order of operations with finite-precision calculations. The USER-INTEL package is deterministic. This means that the results should be reproducible from run to run with the *same* parallel configurations and when using deterministic libraries or library settings (MPI, OpenMP, FFT). However, there are differences in the USER-INTEL package that can change the order of operations compared to LAMMPS without acceleration:

- Neighbor lists can be created in a different order
- Bins used for sorting atoms can be oriented differently
- The default stencil order for PPPM is 7. By default, LAMMPS will calculate other PPPM parameters to fit the desired accuracy with this order
- The *newton* setting applies to all atoms, not just atoms shared between MPI tasks
- Vectorization can change the order for adding pairwise forces
- When using the -DLMP_USE_MKL_RNG define (all included intel optimized makefiles do) at build time, the random number generator for dissipative particle dynamics (pair style dpd/intel) uses the Mersenne Twister generator included in the Intel MKL library (that should be more robust than the default Masaglia random number generator)

The precision mode (described below) used with the USER-INTEL package can change the *accuracy* of the calculations. For the default *mixed* precision option, calculations between pairs or triplets of atoms are performed in single precision, intended to be within the inherent error of MD simulations. All accumulation is performed in double precision to prevent the error from growing with the number of atoms in the simulation. *Single* precision mode should not be used without appropriate validation.

Quick Start for Experienced Users:

LAMMPS should be built with the USER-INTEL package installed. Simulations should be run with 1 MPI task per physical *core*, not *hardware thread*.

- Edit src/MAKE/OPTIONS/Makefile.intel_cpu_intelmpi as necessary.
- Set the environment variable KMP_BLOCKTIME=0
- "-pk intel 0 omp $t -sf intel" added to LAMMPS command-line
- $t should be 2 for Intel Xeon CPUs and 2 or 4 for Intel Xeon Phi
- For some of the simple 2-body potentials without long-range electrostatics, performance and scalability can be better with the "newton off" setting added to the input script
- For simulations on higher node counts, add "processors * * * grid numa" to the beginning of the input script for better scalability
- If using *kspace_style pppm* in the input script, add "kspace_modify diff ad" for better performance

For Intel Xeon Phi CPUs:

- Runs should be performed using MCDRAM.

For simulations using *kspace_style pppm* on Intel CPUs supporting AVX-512:

- Add "kspace_modify diff ad" to the input script
- The command-line option should be changed to "-pk intel 0 omp $r lrt yes -sf intel" where $r is the number of threads minus 1.
- Do not use thread affinity (set KMP_AFFINITY=none)
- The "newton off" setting may provide better scalability

For Intel Xeon Phi co-processors (Offload):

- Edit src/MAKE/OPTIONS/Makefile.intel_co-processor as necessary
- "-pk intel N omp 1" added to command-line where N is the number of co-processors per node.

Required hardware/software:

In order to use offload to co-processors, an Intel Xeon Phi co-processor and an Intel compiler are required. For this, the recommended version of the Intel compiler is 14.0.1.106 or versions 15.0.2.044 and higher.

Although any compiler can be used with the USER-INTEL package, currently, vectorization directives are disabled by default when not using Intel compilers due to lack of standard support and observations of decreased performance. The OpenMP standard now supports directives for vectorization and we plan to transition the code to this standard once it is available in most compilers. We expect this to allow improved performance and support with other compilers.

For Intel Xeon Phi x200 series processors (code-named Knights Landing), there are multiple configuration options for the hardware. For best performance, we recommend that the MCDRAM is configured in "Flat" mode and with the cluster mode set to "Quadrant" or "SNC4". "Cache" mode can also be used, although the performance might be slightly lower.

Notes about Simultaneous Multithreading:

Modern CPUs often support Simultaneous Multithreading (SMT). On Intel processors, this is called Hyper-Threading (HT) technology. SMT is hardware support for running multiple threads efficiently on a single core. *Hardware threads* or *logical cores* are often used to refer to the number of threads that are supported in hardware. For example, the Intel Xeon E5-2697v4 processor is described as having 36 cores and 72 threads. This means that 36 MPI processes or

OpenMP threads can run simultaneously on separate cores, but that up to 72 MPI processes or OpenMP threads can be running on the CPU without costly operating system context switches.

Molecular dynamics simulations will often run faster when making use of SMT. If a thread becomes stalled, for example because it is waiting on data that has not yet arrived from memory, another thread can start running so that the CPU pipeline is still being used efficiently. Although benefits can be seen by launching a MPI task for every hardware thread, for multinode simulations, we recommend that OpenMP threads are used for SMT instead, either with the USER-INTEL package, *USER-OMP package*, or *KOKKOS package*. In the example above, up to 36X speedups can be observed by using all 36 physical cores with LAMMPS. By using all 72 hardware threads, an additional 10-30% performance gain can be achieved.

The BIOS on many platforms allows SMT to be disabled, however, we do not recommend this on modern processors as there is little to no benefit for any software package in most cases. The operating system will report every hardware thread as a separate core allowing one to determine the number of hardware threads available. On Linux systems, this information can normally be obtained with:

```
cat /proc/cpuinfo
```

Building LAMMPS with the USER-INTEL package:

See the *Build extras* doc page for instructions. Some additional details are covered here.

For building with make, several example Makefiles for building with the Intel compiler are included with LAMMPS in the src/MAKE/OPTIONS/ directory:

```
Makefile.intel_cpu_intelmpi # Intel Compiler, Intel MPI, No Offload
Makefile.knl                # Intel Compiler, Intel MPI, No Offload
Makefile.intel_cpu_mpich    # Intel Compiler, MPICH, No Offload
Makefile.intel_cpu_openpmi  # Intel Compiler, OpenMPI, No Offload
Makefile.intel_co-processor  # Intel Compiler, Intel MPI, Offload
```

Makefile.knl is identical to Makefile.intel_cpu_intelmpi except that it explicitly specifies that vectorization should be for Intel Xeon Phi x200 processors making it easier to cross-compile. For users with recent installations of Intel Parallel Studio, the process can be as simple as:

```
make yes-user-intel
source /opt/intel/parallel_studio_xe_2016.3.067/psxevars.sh
# or psxevars.csh for C-shell
make intel_cpu_intelmpi
```

Note that if you build with support for a Phi co-processor, the same binary can be used on nodes with or without co-processors installed. However, if you do not have co-processors on your system, building without offload support will produce a smaller binary.

The general requirements for Makefiles with the USER-INTEL package are as follows. When using Intel compilers, "-restrict" is required and "-qopenmp" is highly recommended for CCFLAGS and LINKFLAGS. CCFLAGS should include "-DLMP_INTEL_USELRT" (unless POSIX Threads are not supported in the build environment) and "-DLMP_USE_MKL_RNG" (unless Intel Math Kernel Library (MKL) is not available in the build environment). For Intel compilers, LIB should include "-ltbbmalloc" or if the library is not available, "-DLMP_INTEL_NO_TBB" can be added to CCFLAGS. For builds supporting offload, "-DLMP_INTEL_OFFLOAD" is required for CCFLAGS and "-qoffload" is required for LINKFLAGS. Other recommended CCFLAG options for best performance are "-O2 -fno-alias -ansi-alias -qoverride-limits fp-model fast=2 -no-prec-div".

Note: See the src/USER-INTEL/README file for additional flags that might be needed for best performance on Intel server processors code-named "Skylake".

Note: The vectorization and math capabilities can differ depending on the CPU. For Intel compilers, the "-x" flag specifies the type of processor for which to optimize. "-xHost" specifies that the compiler should build for the processor used for compiling. For Intel Xeon Phi x200 series processors, this option is "-xMIC-AVX512". For fourth generation Intel Xeon (v4/Broadwell) processors, "-xCORE-AVX2" should be used. For older Intel Xeon processors, "-xAVX" will perform best in general for the different simulations in LAMMPS. The default in most of the example Makefiles is to use "-xHost", however this should not be used when cross-compiling.

Running LAMMPS with the USER-INTEL package:

Running LAMMPS with the USER-INTEL package is similar to normal use with the exceptions that one should 1) specify that LAMMPS should use the USER-INTEL package, 2) specify the number of OpenMP threads, and 3) optionally specify the specific LAMMPS styles that should use the USER-INTEL package. 1) and 2) can be performed from the command-line or by editing the input script. 3) requires editing the input script. Advanced performance tuning options are also described below to get the best performance.

When running on a single node (including runs using offload to a co-processor), best performance is normally obtained by using 1 MPI task per physical core and additional OpenMP threads with SMT. For Intel Xeon processors, 2 OpenMP threads should be used for SMT. For Intel Xeon Phi CPUs, 2 or 4 OpenMP threads should be used (best choice depends on the simulation). In cases where the user specifies that LRT mode is used (described below), 1 or 3 OpenMP threads should be used. For multi-node runs, using 1 MPI task per physical core will often perform best, however, depending on the machine and scale, users might get better performance by decreasing the number of MPI tasks and using more OpenMP threads. For performance, the product of the number of MPI tasks and OpenMP threads should not exceed the number of available hardware threads in almost all cases.

Note: Setting core affinity is often used to pin MPI tasks and OpenMP threads to a core or group of cores so that memory access can be uniform. Unless disabled at build time, affinity for MPI tasks and OpenMP threads on the host (CPU) will be set by default on the host *when using offload to a co-processor*. In this case, it is unnecessary to use other methods to control affinity (e.g. taskset, numactl, I_MPI_PIN_DOMAIN, etc.). This can be disabled with the *no_affinity* option to the *package intel* command or by disabling the option at build time (by adding -DINTEL_OFFLOAD_NOAFFINITY to the CCFLAGS line of your Makefile). Disabling this option is not recommended, especially when running on a machine with Intel Hyper-Threading technology disabled.

Run with the USER-INTEL package from the command line:

To enable USER-INTEL optimizations for all available styles used in the input script, the "-sf intel" *command-line switch* can be used without any requirement for editing the input script. This switch will automatically append "intel" to styles that support it. It also invokes a default command: *package intel 1*. This package command is used to set options for the USER-INTEL package. The default package command will specify that USER-INTEL calculations are performed in mixed precision, that the number of OpenMP threads is specified by the OMP_NUM_THREADS environment variable, and that if co-processors are present and the binary was built with offload support, that 1 co-processor per node will be used with automatic balancing of work between the CPU and the co-processor.

You can specify different options for the USER-INTEL package by using the "-pk intel Nphi" *command-line switch* with keyword/value pairs as specified in the documentation. Here, Nphi = # of Xeon Phi co-processors/node (ignored without offload support). Common options to the USER-INTEL package include *omp* to override any OMP_NUM_THREADS setting and specify the number of OpenMP threads, *mode* to set the floating-point precision mode, and *lrt* to enable Long-Range Thread mode as described below. See the *package intel* command for details, including the default values used for all its options if not specified, and how to set the number of OpenMP threads via the OMP_NUM_THREADS environment variable if desired.

Examples (see documentation for your MPI/Machine for differences in launching MPI applications):

```
mpirun -np 72 -ppn 36 lmp_machine -sf intel -in in.script
↪    # 2 nodes, 36 MPI tasks/node, $OMP_NUM_THREADS OpenMP Threads
mpirun -np 72 -ppn 36 lmp_machine -sf intel -in in.script -pk intel 0 omp 2 mode␣
↪double   # Don't use any co-processors that might be available, use 2 OpenMP␣
↪threads for each task, use double precision
```

Or run with the USER-INTEL package by editing an input script:

As an alternative to adding command-line arguments, the input script can be edited to enable the USER-INTEL package. This requires adding the *package intel* command to the top of the input script. For the second example above, this would be:

```
package intel 0 omp 2 mode double
```

To enable the USER-INTEL package only for individual styles, you can add an "intel" suffix to the individual style, e.g.:

```
pair_style lj/cut/intel 2.5
```

Alternatively, the *suffix intel* command can be added to the input script to enable USER-INTEL styles for the commands that follow in the input script.

Tuning for Performance:

Note: The USER-INTEL package will perform better with modifications to the input script when *PPPM* is used: *kspace_modify diff ad* should be added to the input script.

Long-Range Thread (LRT) mode is an option to the *package intel* command that can improve performance when using *PPPM* for long-range electrostatics on processors with SMT. It generates an extra pthread for each MPI task. The thread is dedicated to performing some of the PPPM calculations and MPI communications. This feature requires setting the pre-processor flag -DLMP_INTEL_USELRT in the makefile when compiling LAMMPS. It is unset in the default makefiles (*Makefile.mpi* and *Makefile.serial*) but it is set in all makefiles tuned for the USER-INTEL package. On Intel Xeon Phi x200 series CPUs, the LRT feature will likely improve performance, even on a single node. On Intel Xeon processors, using this mode might result in better performance when using multiple nodes, depending on the specific machine configuration. To enable LRT mode, specify that the number of OpenMP threads is one less than would normally be used for the run and add the "lrt yes" option to the "-pk" command-line suffix or "package intel" command. For example, if a run would normally perform best with "-pk intel 0 omp 4", instead use "-pk intel 0 omp 3 lrt yes". When using LRT, you should set the environment variable "KMP_AFFINITY=none". LRT mode is not supported when using offload.

Note: Changing the *newton* setting to off can improve performance and/or scalability for simple 2-body potentials such as lj/cut or when using LRT mode on processors supporting AVX-512.

Not all styles are supported in the USER-INTEL package. You can mix the USER-INTEL package with styles from the *OPT* package or the *USER-OMP package*. Of course, this requires that these packages were installed at build time. This can performed automatically by using "-sf hybrid intel opt" or "-sf hybrid intel omp" command-line options. Alternatively, the "opt" and "omp" suffixes can be appended manually in the input script. For the latter, the *package omp* command must be in the input script or the "-pk omp Nt" *command-line switch* must be used where Nt is the number of OpenMP threads. The number of OpenMP threads should not be set differently for the different packages. Note that the *suffix hybrid intel omp* command can also be used within the input script to automatically append the "omp" suffix to styles when USER-INTEL styles are not available.

Note: For simulations on higher node counts, add *processors * * * grid numa* to the beginning of the input script for

better scalability.

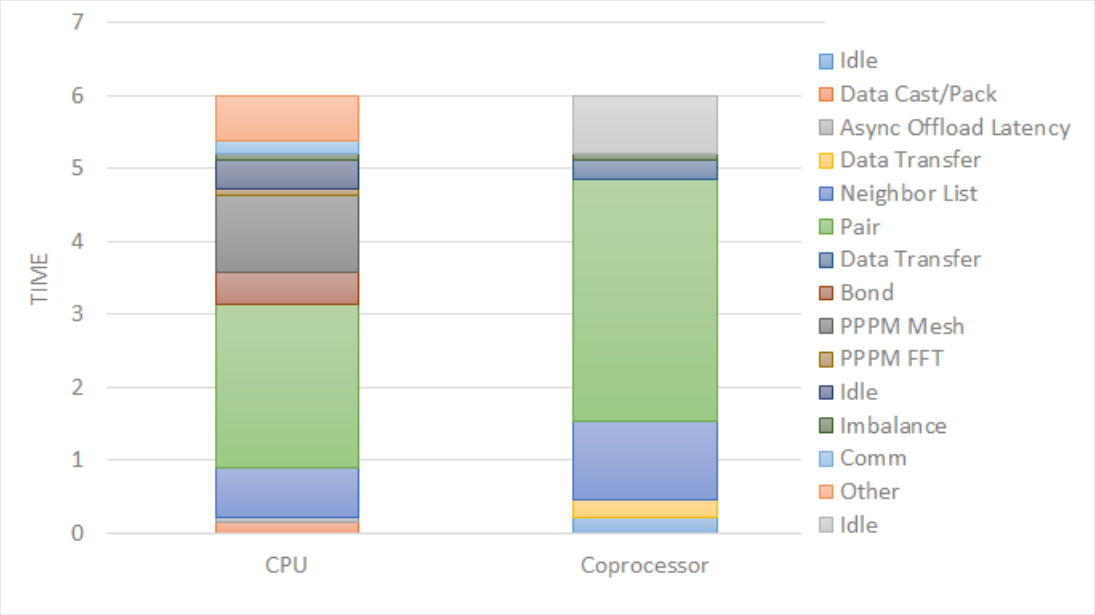
When running on many nodes, performance might be better when using fewer OpenMP threads and more MPI tasks. This will depend on the simulation and the machine. Using the *verlet/split* run style might also give better performance for simulations with *PPPM* electrostatics. Note that this is an alternative to LRT mode and the two cannot be used together.

Currently, when using Intel MPI with Intel Xeon Phi x200 series CPUs, better performance might be obtained by setting the environment variable "I_MPI_SHM_LMT=shm" for Linux kernels that do not yet have full support for AVX-512. Runs on Intel Xeon Phi x200 series processors will always perform better using MCDRAM. Please consult your system documentation for the best approach to specify that MPI runs are performed in MCDRAM.

Tuning for Offload Performance:

The default settings for offload should give good performance.

When using LAMMPS with offload to Intel co-processors, best performance will typically be achieved with concurrent calculations performed on both the CPU and the co-processor. This is achieved by offloading only a fraction of the neighbor and pair computations to the co-processor or using *hybrid* pair styles where only one style uses the "intel" suffix. For simulations with long-range electrostatics or bond, angle, dihedral, improper calculations, computation and data transfer to the co-processor will run concurrently with computations and MPI communications for these calculations on the host CPU. This is illustrated in the figure below for the rhodopsin protein benchmark running on E5-2697v2 processors with a Intel Xeon Phi 7120p co-processor. In this plot, the vertical access is time and routines running at the same time are running concurrently on both the host and the co-processor.



The fraction of the offloaded work is controlled by the *balance* keyword in the *package intel* command. A balance of 0 runs all calculations on the CPU. A balance of 1 runs all supported calculations on the co-processor. A balance of 0.5 runs half of the calculations on the co-processor. Setting the balance to -1 (the default) will enable dynamic load balancing that continuously adjusts the fraction of offloaded work throughout the simulation. Because data transfer cannot be timed, this option typically produces results within 5 to 10 percent of the optimal fixed balance.

If running short benchmark runs with dynamic load balancing, adding a short warm-up run (10-20 steps) will allow the load-balancer to find a near-optimal setting that will carry over to additional runs.

The default for the *package intel* command is to have all the MPI tasks on a given compute node use a single Xeon Phi co-processor. In general, running with a large number of MPI tasks on each node will perform best with offload. Each MPI task will automatically get affinity to a subset of the hardware threads available on the co-processor. For

example, if your card has 61 cores, with 60 cores available for offload and 4 hardware threads per core (240 total threads), running with 24 MPI tasks per node will cause each MPI task to use a subset of 10 threads on the co-processor. Fine tuning of the number of threads to use per MPI task or the number of threads to use per core can be accomplished with keyword settings of the *package intel* command.

The USER-INTEL package has two modes for deciding which atoms will be handled by the co-processor. This choice is controlled with the *ghost* keyword of the *package intel* command. When set to 0, ghost atoms (atoms at the borders between MPI tasks) are not offloaded to the card. This allows for overlap of MPI communication of forces with computation on the co-processor when the *newton* setting is "on". The default is dependent on the style being used, however, better performance may be achieved by setting this option explicitly.

When using offload with CPU Hyper-Threading disabled, it may help performance to use fewer MPI tasks and OpenMP threads than available cores. This is due to the fact that additional threads are generated internally to handle the asynchronous offload tasks.

If pair computations are being offloaded to an Intel Xeon Phi co-processor, a diagnostic line is printed to the screen (not to the log file), during the setup phase of a run, indicating that offload mode is being used and indicating the number of co-processor threads per MPI task. Additionally, an offload timing summary is printed at the end of each run. When offloading, the frequency for *atom sorting* is changed to 1 so that the per-atom data is effectively sorted at every rebuild of the neighbor lists. All the available co-processor threads on each Phi will be divided among MPI tasks, unless the *tptask* option of the "-pk intel" *command-line switch* is used to limit the co-processor threads per MPI task.

Restrictions

When offloading to a co-processor, *hybrid* styles that require skip lists for neighbor builds cannot be offloaded. Using *hybrid/overlay* is allowed. Only one intel accelerated style may be used with hybrid styles when offloading. *Special_bonds* exclusion lists are not currently supported with offload, however, the same effect can often be accomplished by setting cutoffs for excluded atom types to 0. None of the pair styles in the USER-INTEL package currently support the "inner", "middle", "outer" options for rRESPA integration via the *run_style respa* command; only the "pair" option is supported.

References:

- Brown, W.M., Carrillo, J.-M.Y., Mishra, B., Gavhane, N., Thakkar, F.M., De Kraker, A.R., Yamada, M., Ang, J.A., Plimpton, S.J., "Optimizing Classical Molecular Dynamics in LAMMPS," in Intel Xeon Phi Processor High Performance Programming: Knights Landing Edition, J. Jeffers, J. Reinders, A. Sodani, Eds. Morgan Kaufmann.
- Brown, W. M., Semin, A., Hebenstreit, M., Khvostov, S., Raman, K., Plimpton, S.J. Increasing Molecular Dynamics Simulation Rates with an 8-Fold Increase in Electrical Power Efficiency. 2016 High Performance Computing, Networking, Storage and Analysis, SC16: International Conference (pp. 82-95).
- Brown, W.M., Carrillo, J.-M.Y., Gavhane, N., Thakkar, F.M., Plimpton, S.J. Optimizing Legacy Molecular Dynamics Software with Directive-Based Offload. Computer Physics Communications. 2015. 195: p. 95-101.

7.4.3 KOKKOS package

Kokkos is a templated C++ library that provides abstractions to allow a single implementation of an application kernel (e.g. a pair style) to run efficiently on different kinds of hardware, such as GPUs, Intel Xeon Phis, or many-core CPUs. Kokkos maps the C++ kernel onto different back end languages such as CUDA, OpenMP, or Pthreads. The Kokkos library also provides data abstractions to adjust (at compile time) the memory layout of data structures like 2d and 3d arrays to optimize performance on different hardware. For more information on Kokkos, see GitHub. Kokkos is part of Trilinos. The Kokkos library was written primarily by Carter Edwards, Christian Trott, and Dan Sunderland (all Sandia).

The LAMMPS KOKKOS package contains versions of pair, fix, and atom styles that use data structures and macros provided by the Kokkos library, which is included with LAMMPS in /lib/kokkos. The KOKKOS package was developed primarily by Christian Trott (Sandia) and Stan Moore (Sandia) with contributions of various styles by others, including Sikandar Mashayak (UIUC), Ray Shan (Sandia), and Dan Ibanez (Sandia). For more information on developing using Kokkos abstractions see the Kokkos programmers' guide at /lib/kokkos/doc/Kokkos_PG.pdf.

Kokkos currently provides support for 3 modes of execution (per MPI task). These are Serial (MPI-only for CPUs and Intel Phi), OpenMP (threading for many-core CPUs and Intel Phi), and CUDA (for NVIDIA GPUs). You choose the mode at build time to produce an executable compatible with specific hardware.

Note: Kokkos support within LAMMPS must be built with a C++11 compatible compiler. This means GCC version 4.7.2 or later, Intel 14.0.4 or later, or Clang 3.5.2 or later is required.

Note: To build with Kokkos support for NVIDIA GPUs, NVIDIA CUDA software version 7.5 or later must be installed on your system. See the discussion for the *GPU package* for details of how to check and do this.

Note: Kokkos with CUDA currently implicitly assumes that the MPI library is CUDA-aware. This is not always the case, especially when using pre-compiled MPI libraries provided by a Linux distribution. This is not a problem when using only a single GPU with a single MPI rank. When running with multiple MPI ranks, you may see segmentation faults without CUDA-aware MPI support. These can be avoided by adding the flags *-pk kokkos cuda/aware off* to the LAMMPS command line or by using the command *package kokkos cuda/aware off* in the input file.

Building LAMMPS with the KOKKOS package:

See the *Build extras* doc page for instructions.

Running LAMMPS with the KOKKOS package:

All Kokkos operations occur within the context of an individual MPI task running on a single node of the machine. The total number of MPI tasks used by LAMMPS (one or multiple per compute node) is set in the usual manner via the mpirun or mpiexec commands, and is independent of Kokkos. E.g. the mpirun command in OpenMPI does this via its -np and -npernode switches. Ditto for MPICH via -np and -ppn.

Running on a multi-core CPU:

Here is a quick overview of how to use the KOKKOS package for CPU acceleration, assuming one or more 16-core nodes.

```
mpirun -np 16 lmp_kokkos_mpi_only -k on -sf kk -in in.lj        # 1 node, 16 MPI␣
↪tasks/node, no multi-threading
mpirun -np 2 -ppn 1 lmp_kokkos_omp -k on t 16 -sf kk -in in.lj  # 2 nodes, 1 MPI task/
↪node, 16 threads/task
mpirun -np 2 lmp_kokkos_omp -k on t 8 -sf kk -in in.lj          # 1 node,  2 MPI␣
↪tasks/node, 8 threads/task
mpirun -np 32 -ppn 4 lmp_kokkos_omp -k on t 4 -sf kk -in in.lj  # 8 nodes, 4 MPI␣
↪tasks/node, 4 threads/task
```

To run using the KOKKOS package, use the "-k on", "-sf kk" and "-pk kokkos" *command-line switches* in your mpirun command. You must use the "-k on" *command-line switch* to enable the KOKKOS package. It takes additional arguments for hardware settings appropriate to your system. For OpenMP use:

```
-k on t Nt
```

The "t Nt" option specifies how many OpenMP threads per MPI task to use with a node. The default is Nt = 1, which is MPI-only mode. Note that the product of MPI tasks * OpenMP threads/task should not exceed the physical number of cores (on a node), otherwise performance will suffer. If Hyper-Threading (HT) is enabled, then the product of MPI tasks * OpenMP threads/task should not exceed the physical number of cores * hardware threads. The "-k on" switch also issues a "package kokkos" command (with no additional arguments) which sets various KOKKOS options to default values, as discussed on the *package* command doc page.

The "-sf kk" *command-line switch* will automatically append the "/kk" suffix to styles that support it. In this manner no modification to the input script is needed. Alternatively, one can run with the KOKKOS package by editing the input script as described below.

Note: When using a single OpenMP thread, the Kokkos Serial back end (i.e. Makefile.kokkos_mpi_only) will give better performance than the OpenMP back end (i.e. Makefile.kokkos_omp) because some of the overhead to make the code thread-safe is removed.

Note: Use the "-pk kokkos" *command-line switch* to change the default *package kokkos* options. See its doc page for details and default settings. Experimenting with its options can provide a speed-up for specific calculations. For example:

```
mpirun -np 16 lmp_kokkos_mpi_only -k on -sf kk -pk kokkos newton on neigh half comm␣
↪no -in in.lj       # Newton on, Half neighbor list, non-threaded comm
```

If the *newton* command is used in the input script, it can also override the Newton flag defaults.

For half neighbor lists and OpenMP, the KOKKOS package uses data duplication (i.e. thread-private arrays) by default to avoid thread-level write conflicts in the force arrays (and other data structures as necessary). Data duplication is typically fastest for small numbers of threads (i.e. 8 or less) but does increase memory footprint and is not scalable to large numbers of threads. An alternative to data duplication is to use thread-level atomic operations which do not require data duplication. The use of atomic operations can be enforced by compiling LAMMPS with the "-DLMP_KOKKOS_USE_ATOMICS" pre-processor flag. Most but not all Kokkos-enabled pair_styles support data duplication. Alternatively, full neighbor lists avoid the need for duplication or atomic operations but require more compute operations per atom. When using the Kokkos Serial back end or the OpenMP back end with a single thread, no duplication or atomic operations are used. For CUDA and half neighbor lists, the KOKKOS package always uses atomic operations.

Core and Thread Affinity:

When using multi-threading, it is important for performance to bind both MPI tasks to physical cores, and threads to physical cores, so they do not migrate during a simulation.

If you are not certain MPI tasks are being bound (check the defaults for your MPI installation), binding can be forced with these flags:

```
OpenMPI 1.8: mpirun -np 2 --bind-to socket --map-by socket ./lmp_openmpi ...
Mvapich2 2.0: mpiexec -np 2 --bind-to socket --map-by socket ./lmp_mvapich ...
```

For binding threads with KOKKOS OpenMP, use thread affinity environment variables to force binding. With OpenMP 3.1 (gcc 4.7 or later, intel 12 or later) setting the environment variable OMP_PROC_BIND=true should be sufficient. In general, for best performance with OpenMP 4.0 or better set OMP_PROC_BIND=spread and OMP_PLACES=threads. For binding threads with the KOKKOS pthreads option, compile LAMMPS the KOKKOS HWLOC=yes option as described below.

Running on Knight's Landing (KNL) Intel Xeon Phi:

Here is a quick overview of how to use the KOKKOS package for the Intel Knight's Landing (KNL) Xeon Phi:

KNL Intel Phi chips have 68 physical cores. Typically 1 to 4 cores are reserved for the OS, and only 64 or 66 cores are used. Each core has 4 Hyper-Threads,so there are effectively N = 256 (4*64) or N = 264 (4*66) cores to run on. The product of MPI tasks * OpenMP threads/task should not exceed this limit, otherwise performance will suffer. Note that with the KOKKOS package you do not need to specify how many KNLs there are per node; each KNL is simply treated as running some number of MPI tasks.

Examples of mpirun commands that follow these rules are shown below.

```
Intel KNL node with 68 cores (272 threads/node via 4x hardware threading):
mpirun -np 64 lmp_kokkos_phi -k on t 4 -sf kk -in in.lj      # 1 node, 64 MPI tasks/
↪node, 4 threads/task
mpirun -np 66 lmp_kokkos_phi -k on t 4 -sf kk -in in.lj      # 1 node, 66 MPI tasks/
↪node, 4 threads/task
mpirun -np 32 lmp_kokkos_phi -k on t 8 -sf kk -in in.lj      # 1 node, 32 MPI tasks/
↪node, 8 threads/task
mpirun -np 512 -ppn 64 lmp_kokkos_phi -k on t 4 -sf kk -in in.lj  # 8 nodes, 64 MPI␣
↪tasks/node, 4 threads/task
```

The -np setting of the mpirun command sets the number of MPI tasks/node. The "-k on t Nt" command-line switch sets the number of threads/task as Nt. The product of these two values should be N, i.e. 256 or 264.

Note: The default for the *package kokkos* command when running on KNL is to use "half" neighbor lists and set the Newton flag to "on" for both pairwise and bonded interactions. This will typically be best for many-body potentials. For simpler pair-wise potentials, it may be faster to use a "full" neighbor list with Newton flag to "off". Use the "-pk kokkos" *command-line switch* to change the default *package kokkos* options. See its doc page for details and default settings. Experimenting with its options can provide a speed-up for specific calculations. For example:

```
mpirun -np 64 lmp_kokkos_phi -k on t 4 -sf kk -pk kokkos comm host -in in.reax      #␣
↪ Newton on, half neighbor list, threaded comm
mpirun -np 64 lmp_kokkos_phi -k on t 4 -sf kk -pk kokkos newton off neigh full comm␣
↪no -in in.lj      # Newton off, full neighbor list, non-threaded comm
```

Note: MPI tasks and threads should be bound to cores as described above for CPUs.

Note: To build with Kokkos support for Intel Xeon Phi co-processors such as Knight's Corner (KNC), your system must be configured to use them in "native" mode, not "offload" mode like the USER-INTEL package supports.

Running on GPUs:

Use the "-k" *command-line switch* to specify the number of GPUs per node. Typically the -np setting of the mpirun command should set the number of MPI tasks/node to be equal to the number of physical GPUs on the node. You can assign multiple MPI tasks to the same GPU with the KOKKOS package, but this is usually only faster if some portions of the input script have not been ported to use Kokkos. In this case, also packing/unpacking communication buffers on the host may give speedup (see the KOKKOS *package* command). Using CUDA MPS is recommended in this scenario.

Using a CUDA-aware MPI library is highly recommended. CUDA-aware MPI use can be avoided by using *-pk kokkos cuda/aware no*. As above for multi-core CPUs (and no GPU), if N is the number of physical cores/node, then the number of MPI tasks/node should not exceed N.

```
-k on g Ng
```

Here are examples of how to use the KOKKOS package for GPUs, assuming one or more nodes, each with two GPUs:

```
mpirun -np 2 lmp_kokkos_cuda_openmpi -k on g 2 -sf kk -in in.lj          # 1 node,
↪2 MPI tasks/node, 2 GPUs/node
mpirun -np 32 -ppn 2 lmp_kokkos_cuda_openmpi -k on g 2 -sf kk -in in.lj  # 16 nodes,
↪2 MPI tasks/node, 2 GPUs/node (32 GPUs total)
```

Note: The default for the *package kokkos* command when running on GPUs is to use "full" neighbor lists and set the Newton flag to "off" for both pairwise and bonded interactions, along with threaded communication. When running on Maxwell or Kepler GPUs, this will typically be best. For Pascal GPUs, using "half" neighbor lists and setting the Newton flag to "on" may be faster. For many pair styles, setting the neighbor binsize equal to twice the CPU default value will give speedup, which is the default when running on GPUs. Use the "-pk kokkos" *command-line switch* to change the default *package kokkos* options. See its doc page for details and default settings. Experimenting with its options can provide a speed-up for specific calculations. For example:

```
mpirun -np 2 lmp_kokkos_cuda_openmpi -k on g 2 -sf kk -pk kokkos newton on neigh half
↪binsize 2.8 -in in.lj      # Newton on, half neighbor list, set binsize = neighbor
↪ghost cutoff
```

Note: For good performance of the KOKKOS package on GPUs, you must have Kepler generation GPUs (or later). The Kokkos library exploits texture cache options not supported by Telsa generation GPUs (or older).

Note: When using a GPU, you will achieve the best performance if your input script does not use fix or compute styles which are not yet Kokkos-enabled. This allows data to stay on the GPU for multiple timesteps, without being copied back to the host CPU. Invoking a non-Kokkos fix or compute, or performing I/O for *thermo* or *dump* output will cause data to be copied back to the CPU incurring a performance penalty.

Note: To get an accurate timing breakdown between time spend in pair, kspace, etc., you must set the environment variable CUDA_LAUNCH_BLOCKING=1. However, this will reduce performance and is not recommended for production runs.

Run with the KOKKOS package by editing an input script:

Alternatively the effect of the "-sf" or "-pk" switches can be duplicated by adding the *package kokkos* or *suffix kk* commands to your input script.

The discussion above for building LAMMPS with the KOKKOS package, the mpirun/mpiexec command, and setting appropriate thread are the same.

You must still use the "-k on" *command-line switch* to enable the KOKKOS package, and specify its additional arguments for hardware options appropriate to your system, as documented above.

You can use the *suffix kk* command, or you can explicitly add a "kk" suffix to individual styles in your input script, e.g.

```
pair_style lj/cut/kk 2.5
```

You only need to use the *package kokkos* command if you wish to change any of its option defaults, as set by the "-k on" *command-line switch*.

Using OpenMP threading and CUDA together (experimental):

With the KOKKOS package, both OpenMP multi-threading and GPUs can be used together in a few special cases. In the Makefile, the KOKKOS_DEVICES variable must include both "Cuda" and "OpenMP", as is the case for

/src/MAKE/OPTIONS/Makefile.kokkos_cuda_mpi

```
KOKKOS_DEVICES=Cuda,OpenMP
```

The suffix "/kk" is equivalent to "/kk/device", and for Kokkos CUDA, using the "-sf kk" in the command line gives the default CUDA version everywhere. However, if the "/kk/host" suffix is added to a specific style in the input script, the Kokkos OpenMP (CPU) version of that specific style will be used instead. Set the number of OpenMP threads as "t Nt" and the number of GPUs as "g Ng"

```
-k on t Nt g Ng
```

For example, the command to run with 1 GPU and 8 OpenMP threads is then:

```
mpiexec -np 1 lmp_kokkos_cuda_openmpi -in in.lj -k on g 1 t 8 -sf kk
```

Conversely, if the "-sf kk/host" is used in the command line and then the "/kk" or "/kk/device" suffix is added to a specific style in your input script, then only that specific style will run on the GPU while everything else will run on the CPU in OpenMP mode. Note that the execution of the CPU and GPU styles will NOT overlap, except for a special case:

A kspace style and/or molecular topology (bonds, angles, etc.) running on the host CPU can overlap with a pair style running on the GPU. First compile with "–default-stream per-thread" added to CCFLAGS in the Kokkos CUDA Makefile. Then explicitly use the "/kk/host" suffix for kspace and bonds, angles, etc. in the input file and the "kk" suffix (equal to "kk/device") on the command line. Also make sure the environment variable CUDA_LAUNCH_BLOCKING is not set to "1" so CPU/GPU overlap can occur.

Speed-ups to expect:

The performance of KOKKOS running in different modes is a function of your hardware, which KOKKOS-enable styles are used, and the problem size.

Generally speaking, the following rules of thumb apply:

- When running on CPUs only, with a single thread per MPI task, performance of a KOKKOS style is somewhere between the standard (un-accelerated) styles (MPI-only mode), and those provided by the USER-OMP package. However the difference between all 3 is small (less than 20%).
- When running on CPUs only, with multiple threads per MPI task, performance of a KOKKOS style is a bit slower than the USER-OMP package.
- When running large number of atoms per GPU, KOKKOS is typically faster than the GPU package.
- When running on Intel hardware, KOKKOS is not as fast as the USER-INTEL package, which is optimized for that hardware.

See the Benchmark page of the LAMMPS web site for performance of the KOKKOS package on different hardware.

Advanced Kokkos options:

There are other allowed options when building with the KOKKOS package. As explained on the *Build extras* doc page, they can be set either as variables on the make command line or in Makefile.machine, or they can be specified as CMake variables. Each takes a value shown below. The default value is listed, which is set in the lib/kokkos/Makefile.kokkos file.

- KOKKOS_DEBUG, values = *yes*, *no*, default = *no*
- KOKKOS_USE_TPLS, values = *hwloc*, *librt*, *experimental_memkind*, default = *none*
- KOKKOS_CXX_STANDARD, values = *c++11*, *c++1z*, default = *c++11*
- KOKKOS_OPTIONS, values = *aggressive_vectorization*, *disable_profiling*, default = *none*
- KOKKOS_CUDA_OPTIONS, values = *force_uvm*, *use_ldg*, *rdc*, *enable_lambda*, default = *enable_lambda*

KOKKOS_USE_TPLS=hwloc binds threads to hardware cores, so they do not migrate during a simulation. KOKKOS_USE_TPLS=hwloc should always be used if running with KOKKOS_DEVICES=Pthreads for pthreads. It is not necessary for KOKKOS_DEVICES=OpenMP for OpenMP, because OpenMP provides alternative methods via environment variables for binding threads to hardware cores. More info on binding threads to cores is given on the *Speed omp* doc page.

KOKKOS_USE_TPLS=librt enables use of a more accurate timer mechanism on most Unix platforms. This library is not available on all platforms.

KOKKOS_DEBUG is only useful when developing a Kokkos-enabled style within LAMMPS. KOKKOS_DEBUG=yes enables printing of run-time debugging information that can be useful. It also enables runtime bounds checking on Kokkos data structures.

KOKKOS_CXX_STANDARD and KOKKOS_OPTIONS are typically not changed when building LAMMPS.

KOKKOS_CUDA_OPTIONS are additional options for CUDA. The LAMMPS KOKKOS package must be compiled with the *enable_lambda* option when using GPUs.

Restrictions

Currently, there are no precision options with the KOKKOS package. All compilation and computation is performed in double precision.

7.4.4 USER-OMP package

The USER-OMP package was developed by Axel Kohlmeyer at Temple University. It provides optimized and multi-threaded versions of many pair styles, nearly all bonded styles (bond, angle, dihedral, improper), several Kspace styles, and a few fix styles. It uses the OpenMP interface for multi-threading, but can also be compiled without OpenMP support, providing optimized serial styles in that case.

Required hardware/software:

To enable multi-threading, your compiler must support the OpenMP interface. You should have one or more multi-core CPUs, as multiple threads can only be launched by each MPI task on the local node (using shared memory).

Building LAMMPS with the USER-OMP package:

See the *Build extras* doc page for instructions.

Run with the USER-OMP package from the command line:

These examples assume one or more 16-core nodes.

```
env OMP_NUM_THREADS=16 lmp_omp -sf omp -in in.script           # 1 MPI task, 16␣
↪threads according to OMP_NUM_THREADS
lmp_mpi -sf omp -in in.script                                  # 1 MPI task, no␣
↪threads, optimized kernels
mpirun -np 4 lmp_omp -sf omp -pk omp 4 -in in.script           # 4 MPI tasks, 4␣
↪threads/task
mpirun -np 32 -ppn 4 lmp_omp -sf omp -pk omp 4 -in in.script   # 8 nodes, 4 MPI tasks/
↪node, 4 threads/task
```

The mpirun or mpiexec command sets the total number of MPI tasks used by LAMMPS (one or multiple per compute node) and the number of MPI tasks used per node. E.g. the mpirun command in MPICH does this via its -np and -ppn switches. Ditto for OpenMPI via -np and -npernode.

You need to choose how many OpenMP threads per MPI task will be used by the USER-OMP package. Note that the product of MPI tasks * threads/task should not exceed the physical number of cores (on a node), otherwise performance will suffer.

As in the lines above, use the "-sf omp" *command-line switch*, which will automatically append "omp" to styles that support it. The "-sf omp" switch also issues a default *package omp 0* command, which will set the number of threads per MPI task via the OMP_NUM_THREADS environment variable.

You can also use the "-pk omp Nt" *command-line switch*, to explicitly set Nt = # of OpenMP threads per MPI task to use, as well as additional options. Its syntax is the same as the *package omp* command whose doc page gives details, including the default values used if it is not specified. It also gives more details on how to set the number of threads via the OMP_NUM_THREADS environment variable.

Or run with the USER-OMP package by editing an input script:

The discussion above for the mpirun/mpiexec command, MPI tasks/node, and threads/MPI task is the same.

Use the *suffix omp* command, or you can explicitly add an "omp" suffix to individual styles in your input script, e.g.

```
pair_style lj/cut/omp 2.5
```

You must also use the *package omp* command to enable the USER-OMP package. When you do this you also specify how many threads per MPI task to use. The command doc page explains other options and how to set the number of threads via the OMP_NUM_THREADS environment variable.

Speed-ups to expect:

Depending on which styles are accelerated, you should look for a reduction in the "Pair time", "Bond time", "KSpace time", and "Loop time" values printed at the end of a run.

You may see a small performance advantage (5 to 20%) when running a USER-OMP style (in serial or parallel) with a single thread per MPI task, versus running standard LAMMPS with its standard un-accelerated styles (in serial or all-MPI parallelization with 1 task/core). This is because many of the USER-OMP styles contain similar optimizations to those used in the OPT package, described in *Section 5.3.5*.

With multiple threads/task, the optimal choice of number of MPI tasks/node and OpenMP threads/task can vary a lot and should always be tested via benchmark runs for a specific simulation running on a specific machine, paying attention to guidelines discussed in the next sub-section.

A description of the multi-threading strategy used in the USER-OMP package and some performance examples are presented here

Guidelines for best performance:

For many problems on current generation CPUs, running the USER-OMP package with a single thread/task is faster than running with multiple threads/task. This is because the MPI parallelization in LAMMPS is often more efficient than multi-threading as implemented in the USER-OMP package. The parallel efficiency (in a threaded sense) also varies for different USER-OMP styles.

Using multiple threads/task can be more effective under the following circumstances:

- Individual compute nodes have a significant number of CPU cores but the CPU itself has limited memory bandwidth, e.g. for Intel Xeon 53xx (Clovertown) and 54xx (Harpertown) quad-core processors. Running one MPI task per CPU core will result in significant performance degradation, so that running with 4 or even only 2 MPI tasks per node is faster. Running in hybrid MPI+OpenMP mode will reduce the inter-node communication bandwidth contention in the same way, but offers an additional speedup by utilizing the otherwise idle CPU cores.
- The interconnect used for MPI communication does not provide sufficient bandwidth for a large number of MPI tasks per node. For example, this applies to running over gigabit ethernet or on Cray XT4 or XT5 series supercomputers. As in the aforementioned case, this effect worsens when using an increasing number of nodes.
- The system has a spatially inhomogeneous particle density which does not map well to the *domain decomposition scheme* or *load-balancing* options that LAMMPS provides. This is because multi-threading achieves parallelism over the number of particles, not via their distribution in space.

- A machine is being used in "capability mode", i.e. near the point where MPI parallelism is maxed out. For example, this can happen when using the *PPPM solver* for long-range electrostatics on large numbers of nodes. The scaling of the KSpace calculation (see the *kspace_style* command) becomes the performance-limiting factor. Using multi-threading allows less MPI tasks to be invoked and can speed-up the long-range solver, while increasing overall performance by parallelizing the pairwise and bonded calculations via OpenMP. Likewise additional speedup can be sometimes be achieved by increasing the length of the Coulombic cutoff and thus reducing the work done by the long-range solver. Using the *run_style verlet/split* command, which is compatible with the USER-OMP package, is an alternative way to reduce the number of MPI tasks assigned to the KSpace calculation.

Additional performance tips are as follows:

- The best parallel efficiency from *omp* styles is typically achieved when there is at least one MPI task per physical CPU chip, i.e. socket or die.
- It is usually most efficient to restrict threading to a single socket, i.e. use one or more MPI task per socket.
- NOTE: By default, several current MPI implementations use a processor affinity setting that restricts each MPI task to a single CPU core. Using multi-threading in this mode will force all threads to share the one core and thus is likely to be counterproductive. Instead, binding MPI tasks to a (multi-core) socket, should solve this issue.

Restrictions

None.

7.4.5 OPT package

The OPT package was developed by James Fischer (High Performance Technologies), David Richie, and Vincent Natoli (Stone Ridge Technologies). It contains a handful of pair styles whose compute() methods were rewritten in C++ templated form to reduce the overhead due to if tests and other conditional code.

Required hardware/software:

None.

Building LAMMPS with the OPT package:

See the *Build extras* doc page for instructions.

Run with the OPT package from the command line:

```
lmp_mpi -sf opt -in in.script                # run in serial
mpirun -np 4 lmp_mpi -sf opt -in in.script   # run in parallel
```

Use the "-sf opt" *command-line switch*, which will automatically append "opt" to styles that support it.

Or run with the OPT package by editing an input script:

Use the *suffix opt* command, or you can explicitly add an "opt" suffix to individual styles in your input script, e.g.

```
pair_style lj/cut/opt 2.5
```

Speed-ups to expect:

You should see a reduction in the "Pair time" value printed at the end of a run. On most machines for reasonable problem sizes, it will be a 5 to 20% savings.

Guidelines for best performance:

Just try out an OPT pair style to see how it performs.

Restrictions

None.

Inverting this list, LAMMPS currently has acceleration support for three kinds of hardware, via the listed packages:

Many-core CPUs	*USER-INTEL*, *KOKKOS*, *USER-OMP*, *OPT* packages
NVIDIA GPUs	*GPU*, *KOKKOS* packages
Intel Phi	*USER-INTEL*, *KOKKOS* packages

Which package is fastest for your hardware may depend on the size problem you are running and what commands (accelerated and non-accelerated) are invoked by your input script. While these doc pages include performance guidelines, there is no substitute for trying out the different packages appropriate to your hardware.

Any accelerated style has the same name as the corresponding standard style, except that a suffix is appended. Otherwise, the syntax for the command that uses the style is identical, their functionality is the same, and the numerical results it produces should also be the same, except for precision and round-off effects.

For example, all of these styles are accelerated variants of the Lennard-Jones *pair_style lj/cut*:

- *pair_style lj/cut/gpu*
- *pair_style lj/cut/intel*
- *pair_style lj/cut/kk*
- *pair_style lj/cut/omp*
- *pair_style lj/cut/opt*

To see what accelerate styles are currently available for a particular style, find the style name in the *Commands* style pages (fix,compute,pair,etc) and see what suffixes are listed (g,i,k,o,t) with it. The doc pages for individual commands (e.g. *pair lj/cut* or *fix nve*) also list any accelerated variants available for that style.

To use an accelerator package in LAMMPS, and one or more of the styles it provides, follow these general steps. Details vary from package to package and are explained in the individual accelerator doc pages, listed above:

build the accelerator library	only for GPU package
install the accelerator package	make yes-opt, make yes-user-intel, etc
add compile/link flags to Makefile.machine in src/MAKE	only for USER-INTEL, KOKKOS, USER-OMP, OPT packages
re-build LAMMPS	make machine
prepare and test a regular LAMMPS simulation	lmp_machine -in in.script; mpirun -np 32 lmp_machine -in in.script
enable specific accelerator support via '-k on' *command-line switch*,	only needed for KOKKOS package
set any needed options for the package via "-pk" *command-line switch* or *package* command,	only if defaults need to be changed
use accelerated styles in your input via "-sf" *command-line switch* or *suffix* command	lmp_machine -in in.script -sf gpu

Note that the first 4 steps can be done as a single command with suitable make command invocations. This is discussed on the *Packages* doc pages, and its use is illustrated in the individual accelerator sections. Typically these steps only need to be done once, to create an executable that uses one or more accelerator packages.

The last 4 steps can all be done from the command-line when LAMMPS is launched, without changing your input script, as illustrated in the individual accelerator sections. Or you can add *package* and *suffix* commands to your input script.

Note: With a few exceptions, you can build a single LAMMPS executable with all its accelerator packages installed. Note however that the USER-INTEL and KOKKOS packages require you to choose one of their hardware options when building for a specific platform. I.e. CPU or Phi option for the USER-INTEL package. Or the OpenMP, Cuda, or Phi option for the KOKKOS package.

These are the exceptions. You cannot build a single executable with:

- both the USER-INTEL Phi and KOKKOS Phi options
- the USER-INTEL Phi or Kokkos Phi option, and the GPU package

See the examples/accelerate/README and make.list files for sample Make.py commands that build LAMMPS with any or all of the accelerator packages. As an example, here is a command that builds with all the GPU related packages installed (GPU, KOKKOS with Cuda), including settings to build the needed auxiliary GPU libraries for Kepler GPUs:

```
Make.py -j 16 -p omp gpu kokkos -cc nvcc wrap=mpi   -gpu mode=double arch=35 -kokkos␣
↪cuda arch=35 lib-all file mpi
```

The examples/accelerate directory also has input scripts that can be used with all of the accelerator packages. See its README file for details.

Likewise, the bench directory has FERMI and KEPLER and PHI sub-directories with Make.py commands and input scripts for using all the accelerator packages on various machines. See the README files in those directories.

As mentioned above, the Benchmark page of the LAMMPS web site gives performance results for the various accelerator packages for several of the standard LAMMPS benchmark problems, as a function of problem size and number of compute nodes, on different hardware platforms.

Here is a brief summary of what the various packages provide. Details are in the individual accelerator sections.

- Styles with a "gpu" suffix are part of the GPU package, and can be run on NVIDIA GPUs. The speed-up on a GPU depends on a variety of factors, discussed in the accelerator sections.
- Styles with an "intel" suffix are part of the USER-INTEL package. These styles support vectorized single and mixed precision calculations, in addition to full double precision. In extreme cases, this can provide speedups over 3.5x on CPUs. The package also supports acceleration in "offload" mode to Intel(R) Xeon Phi(TM) co-processors. This can result in additional speedup over 2x depending on the hardware configuration.
- Styles with a "kk" suffix are part of the KOKKOS package, and can be run using OpenMP on multicore CPUs, on an NVIDIA GPU, or on an Intel Xeon Phi in "native" mode. The speed-up depends on a variety of factors, as discussed on the KOKKOS accelerator page.
- Styles with an "omp" suffix are part of the USER-OMP package and allow a pair-style to be run in multi-threaded mode using OpenMP. This can be useful on nodes with high-core counts when using less MPI processes than cores is advantageous, e.g. when running with PPPM so that FFTs are run on fewer MPI processors or when the many MPI tasks would overload the available bandwidth for communication.
- Styles with an "opt" suffix are part of the OPT package and typically speed-up the pairwise calculations of your simulation by 5-25% on a CPU.

The individual accelerator package doc pages explain:

- what hardware and software the accelerated package requires
- how to build LAMMPS with the accelerated package
- how to run with the accelerated package either via command-line switches or modifying the input script

- speed-ups to expect
- guidelines for best performance
- restrictions

7.5 Comparison of various accelerator packages

The next section compares and contrasts the various accelerator options, since there are multiple ways to perform OpenMP threading, run on GPUs, optimize for vector units on CPUs and run on Intel Xeon Phi (co-)processors.

All of these packages can accelerate a LAMMPS calculation taking advantage of hardware features, but they do it in different ways and acceleration is not always guaranteed.

As a consequence, for a particular simulation on specific hardware, one package may be faster than the other. We give some guidelines below, but the best way to determine which package is faster for your input script is to try multiple of them on your machine and experiment with available performance tuning settings. See the benchmarking section below for examples where this has been done.

Guidelines for using each package optimally:

- Both, the GPU and the KOKKOS package allows you to assign multiple MPI ranks (= CPU cores) to the same GPU. For the GPU package, this can lead to a speedup through better utilization of the GPU (by overlapping computation and data transfer) and more efficient computation of the non-GPU accelerated parts of LAMMPS through MPI parallelization, as all system data is maintained and updated on the host. For KOKKOS, there is less to no benefit from this, due to its different memory management model, which tries to retain data on the GPU.
- The GPU package moves per-atom data (coordinates, forces, and (optionally) neighbor list data, if not computed on the GPU) between the CPU and GPU at every timestep. The KOKKOS/CUDA package only does this on timesteps when a CPU calculation is required (e.g. to invoke a fix or compute that is non-GPU-ized). Hence, if you can formulate your input script to only use GPU-ized fixes and computes, and avoid doing I/O too often (thermo output, dump file snapshots, restart files), then the data transfer cost of the KOKKOS/CUDA package can be very low, causing it to run faster than the GPU package.
- The GPU package is often faster than the KOKKOS/CUDA package, when the number of atoms per GPU is on the smaller side. The crossover point, in terms of atoms/GPU at which the KOKKOS/CUDA package becomes faster depends strongly on the pair style. For example, for a simple Lennard Jones system the crossover (in single precision) is often about 50K-100K atoms per GPU. When performing double precision calculations the crossover point can be significantly smaller.
- Both KOKKOS and GPU package compute bonded interactions (bonds, angles, etc) on the CPU. If the GPU package is running with several MPI processes assigned to one GPU, the cost of computing the bonded interactions is spread across more CPUs and hence the GPU package can run faster in these cases.
- When using LAMMPS with multiple MPI ranks assigned to the same GPU, its performance depends to some extent on the available bandwidth between the CPUs and the GPU. This can differ significantly based on the available bus technology, capability of the host CPU and mainboard, the wiring of the buses and whether switches are used to increase the number of available bus slots, or if GPUs are housed in an external enclosure. This can become quite complex.
- To achieve significant acceleration through GPUs, both KOKKOS and GPU package require capable GPUs with fast on-device memory and efficient data transfer rates. This requests capable upper mid-level to high-end (desktop) GPUs. Using lower performance GPUs (e.g. on laptops) may result in a slowdown instead.
- For the GPU package, specifically when running in parallel with MPI, if it often more efficient to exclude the PPPM kspace style from GPU acceleration and instead run it - concurrently with a GPU accelerated pair style -

on the CPU. This can often be easily achieved with placing a *suffix off* command before and a *suffix on* command after the *kspace_style pppm* command.

- The KOKKOS/OpenMP and USER-OMP package have different thread management strategies, which should result in USER-OMP being more efficient for a small number of threads with increasing overhead as the number of threads per MPI rank grows. The KOKKOS/OpenMP kernels have less overhead in that case, but have lower performance with few threads.
- The USER-INTEL package contains many options and settings for achieving additional performance on Intel hardware (CPU and accelerator cards), but to unlock this potential, an Intel compiler is required. The package code will compile with GNU gcc, but it will not be as efficient.

Differences between the GPU and KOKKOS packages:

- The GPU package accelerates only pair force, neighbor list, and (parts of) PPPM calculations. The KOKKOS package attempts to run most of the calculation on the GPU, but can transparently support non-accelerated code (with a performance penalty due to having data transfers between host and GPU).
- The GPU package requires neighbor lists to be built on the CPU when using exclusion lists, or a triclinic simulation box.
- The GPU package can be compiled for CUDA or OpenCL and thus supports both, Nvidia and AMD GPUs well. On Nvidia hardware, using CUDA is typically resulting in equal or better performance over OpenCL.
- OpenCL in the GPU package does theoretically also support Intel CPUs or Intel Xeon Phi, but the native support for those in KOKKOS (or USER-INTEL) is superior.

CHAPTER

EIGHT

HOWTO DISCUSSIONS

These doc pages describe how to perform various tasks with LAMMPS, both for users and developers. The glossary website page also lists MD terminology with links to corresponding LAMMPS manual pages. The example input scripts included in the examples directory of the LAMMPS distribution and highlighted on the *Examples* doc page also show how to setup and run various kinds of simulations.

8.1 Tutorials howto

8.1.1 LAMMPS GitHub tutorial

written by Stefan Paquay

This document describes the process of how to use GitHub to integrate changes or additions you have made to LAMMPS into the official LAMMPS distribution. It uses the process of updating this very tutorial as an example to describe the individual steps and options. You need to be familiar with git and you may want to have a look at the git book to reacquaint yourself with some of the more advanced git features used below.

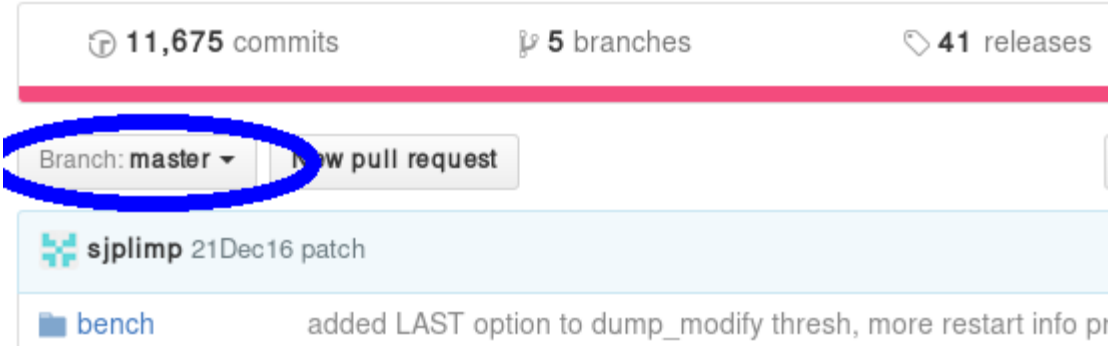
As of fall 2016, submitting contributions to LAMMPS via pull requests on GitHub is the preferred option for integrating contributed features or improvements to LAMMPS, as it significantly reduces the amount of work required by the LAMMPS developers. Consequently, creating a pull request will increase your chances to have your contribution included and will reduce the time until the integration is complete. For more information on the requirements to have your code included into LAMMPS please see the *Modify contribute* doc page.

Making an account

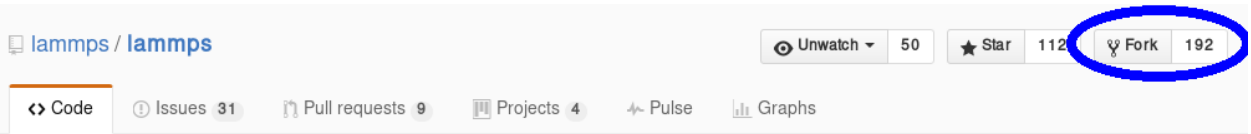
First of all, you need a GitHub account. This is fairly simple, just go to GitHub and create an account by clicking the "Sign up for GitHub" button. Once your account is created, you can sign in by clicking the button in the top left and filling in your username or e-mail address and password.

Forking the repository

To get changes into LAMMPS, you need to first fork the *lammps/lammps* repository on GitHub. At the time of writing, *master* is the preferred target branch. Thus go to LAMMPS on GitHub and make sure branch is set to "master", as shown in the figure below.



If it is not, use the button to change it to *master*. Once it is, use the fork button to create a fork.



This will create a fork (which is essentially a copy, but uses less resources) of the LAMMPS repository under your own GitHub account. You can make changes in this fork and later file *pull requests* to allow the upstream repository to merge changes from your own fork into the one we just forked from (or others that were forked from the same repository). At the same time, you can set things up, so you can include changes from upstream into your repository and thus keep it in sync with the ongoing LAMMPS development.

Adding changes to your own fork

Additions to the upstream version of LAMMPS are handled using *feature branches*. For every new feature, a so-called feature branch is created, which contains only those modification relevant to one specific feature. For example, adding a single fix would consist of creating a branch with only the fix header and source file and nothing else. It is explained in more detail here: feature branch workflow.

Feature branches

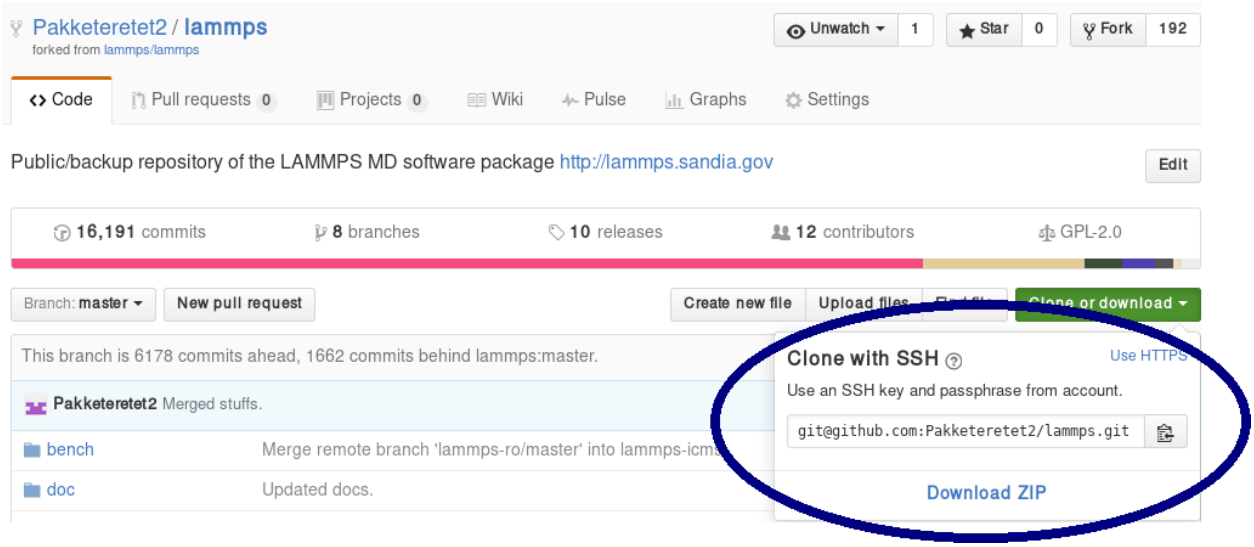
First of all, create a clone of your version on github on your local machine via HTTPS:

```
$ git clone https://github.com/<your user name>/lammps.git <some name>
```

or, if you have set up your GitHub account for using SSH keys, via SSH:

```
$ git clone git@github.com:<your user name>/lammps.git
```

You can find the proper URL by clicking the "Clone or download"-button:



The above command copies ("clones") the git repository to your local machine to a directory with the name you chose. If none is given, it will default to "lammps". Typical names are "mylammps" or something similar.

You can use this local clone to make changes and test them without interfering with the repository on GitHub.

To pull changes from upstream into this copy, you can go to the directory and use git pull:

```
$ cd mylammps
$ git checkout master
$ git pull https://github.com/lammps/lammps
```

You can also add this URL as a remote:

```
$ git remote add lammps_upstream https://www.github.com/lammps/lammps
```

At this point, you typically make a feature branch from the updated master branch for the feature you want to work on. This tutorial contains the workflow that updated this tutorial, and hence we will call the branch "github-tutorial-update":

```
$ git checkout -b github-tutorial-update master
```

Now that we have changed branches, we can make our changes to our local repository. Just remember that if you want to start working on another, unrelated feature, you should switch branches!

After changes are made

After everything is done, add the files to the branch and commit them:

```
$ git add doc/src/Howto_github.txt
$ git add doc/src/JPG/tutorial*.png
```

> **Warning:** Do not use *git commit -a* (or *git add -A*). The -a flag (or -A flag) will automatically include **all** modified **and** new files and that is rarely the behavior you want. It can easily lead to accidentally adding unrelated and unwanted changes into the repository. Instead it is preferable to explicitly use *git add*, *git rm*, *git mv* for adding, removing, renaming individual files, respectively, and then *git commit* to finalize the commit. Carefully check all pending changes with *git status* before committing them. If you find doing this on the command line too tedious, consider using a GUI, for example the one included in git distributions written in Tk, i.e. use *git gui* (on some Linux distributions it may be required to install an additional package to use it).

After adding all files, the change set can be committed with some useful message that explains the change.

```
$ git commit -m 'Finally updated the github tutorial'
```

After the commit, the changes can be pushed to the same branch on GitHub:

```
$ git push
```

Git will ask you for your user name and password on GitHub if you have not configured anything. If your local branch is not present on GitHub yet, it will ask you to add it by running

```
$ git push --set-upstream origin github-tutorial-update
```

If you correctly type your user name and password, the feature branch should be added to your fork on GitHub.

If you want to make really sure you push to the right repository (which is good practice), you can provide it explicitly:

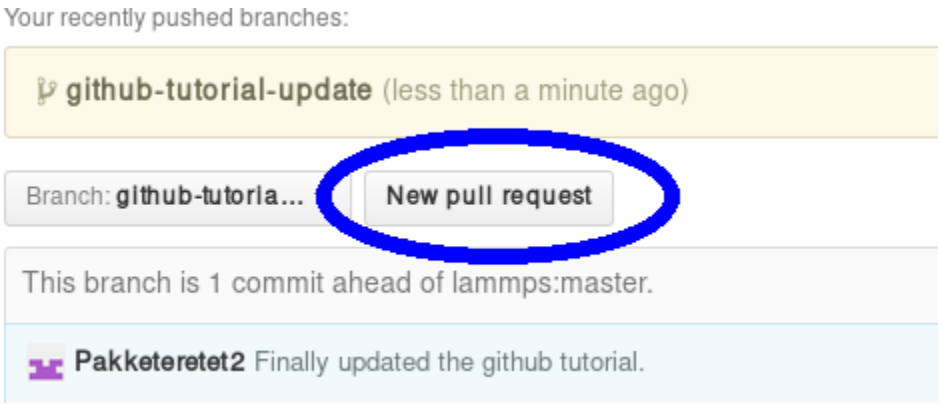
```
$ git push origin
```

or using an explicit URL:

```
$ git push git@github.com:Pakketeretet2/lammps.git
```

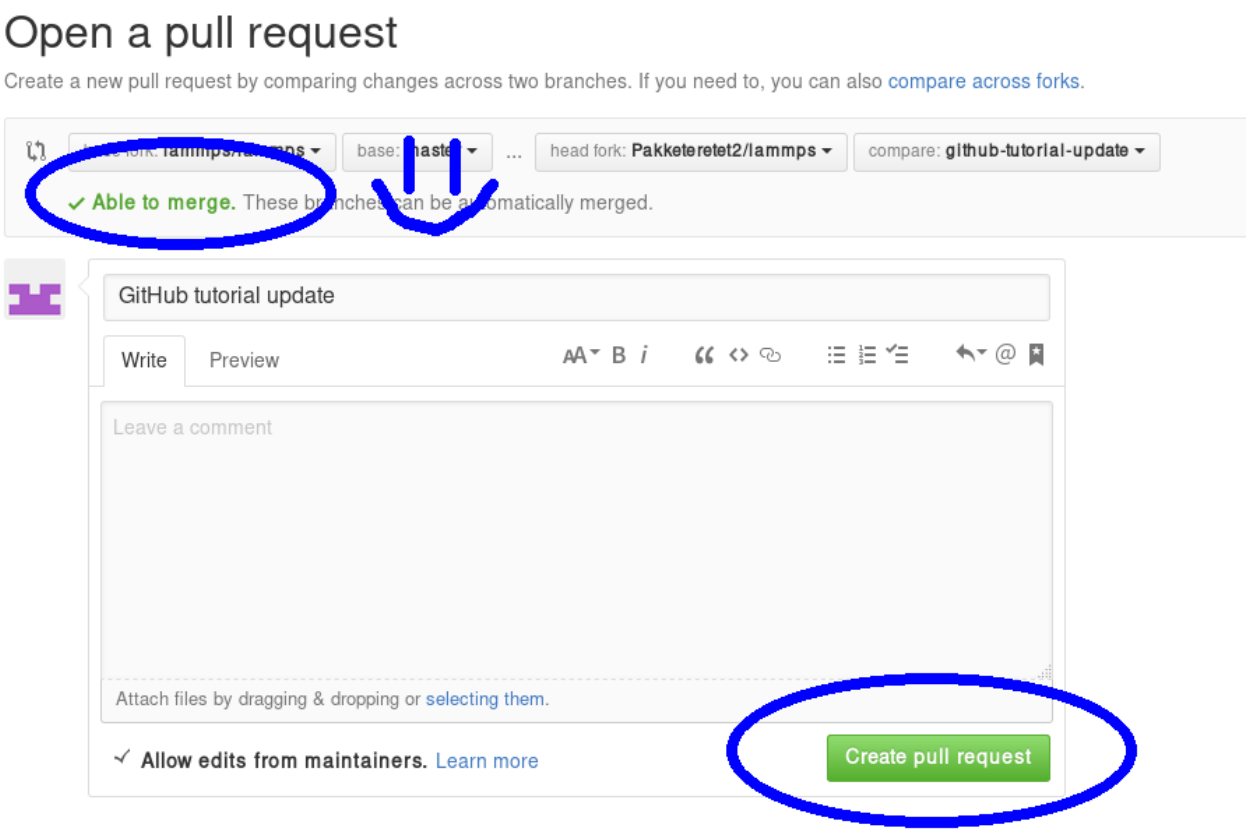
Filing a pull request

Up to this point in the tutorial, all changes were to *your* clones of LAMMPS. Eventually, however, you want this feature to be included into the official LAMMPS version. To do this, you will want to file a pull request by clicking on the "New pull request" button:



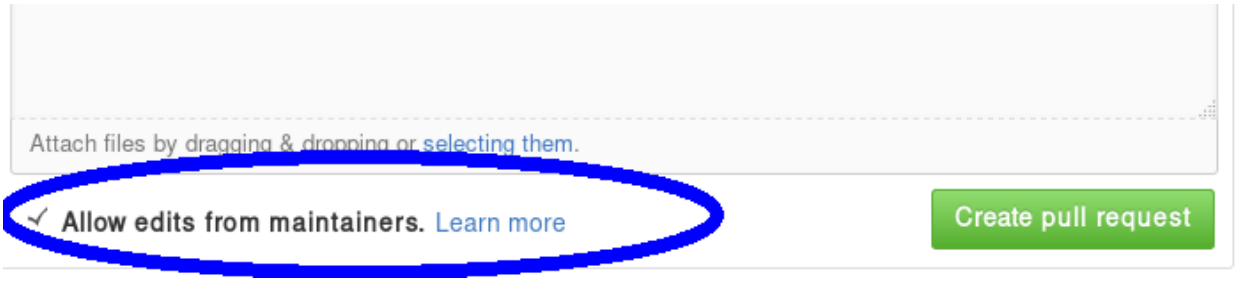
Make sure that the current branch is set to the correct one, which, in this case, is "github-tutorial-update". If done correctly, the only changes you will see are those that were made on this branch.

This will open up a new window that lists changes made to the repository. If you are just adding new files, there is not much to do, but I suppose merge conflicts are to be resolved here if there are changes in existing files. If all changes can automatically be merged, green text at the top will say so and you can click the "Create pull request" button, see image.



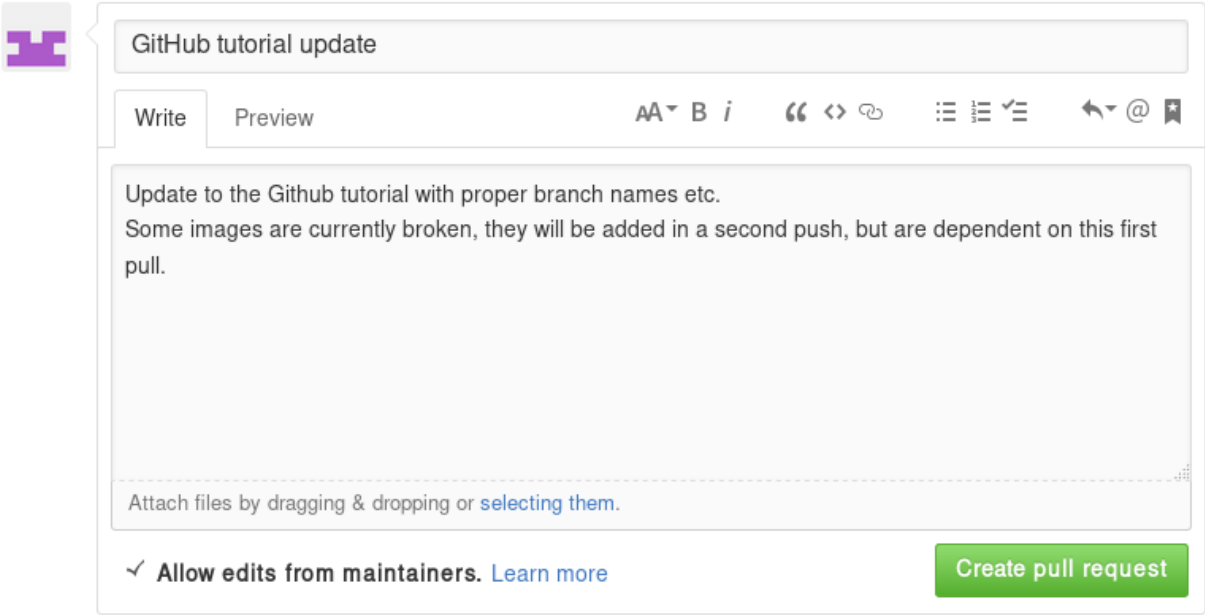
Before creating the pull request, make sure the short title is accurate and add a comment with details about your pull request. Here you write what your modifications do and why they should be incorporated upstream.

Note the checkbox that says "Allow edits from maintainers". This is checked by default checkbox (although in my version of Firefox, only the checkmark is visible):



If it is checked, maintainers can immediately add their own edits to the pull request. This helps the inclusion of your branch significantly, as simple/trivial changes can be added directly to your pull request branch by the LAMMPS maintainers. The alternative would be that they make changes on their own version of the branch and file a reverse pull request to you. Just leave this box checked unless you have a very good reason not to.

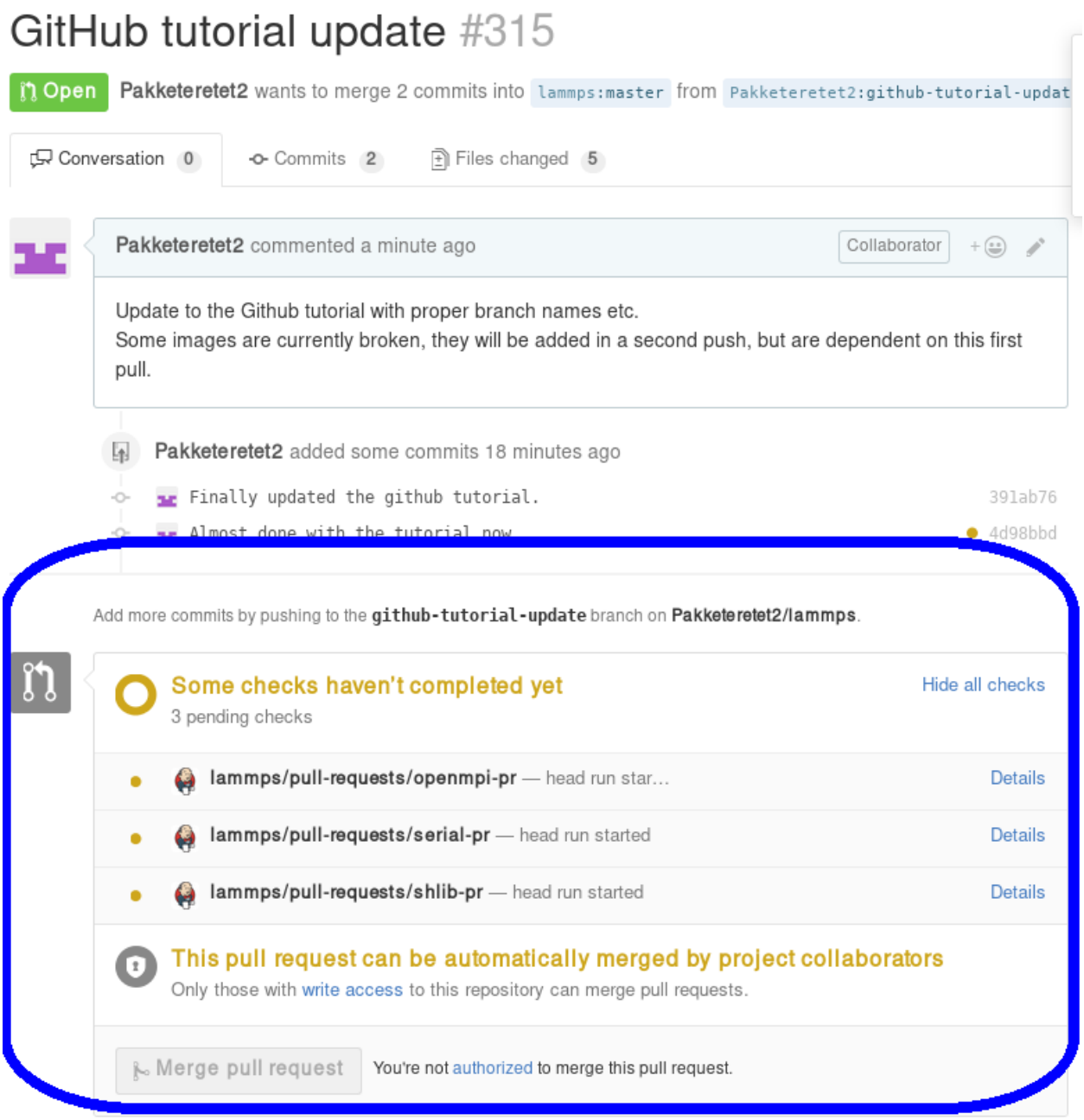
Now just write some nice comments and click on "Create pull request".



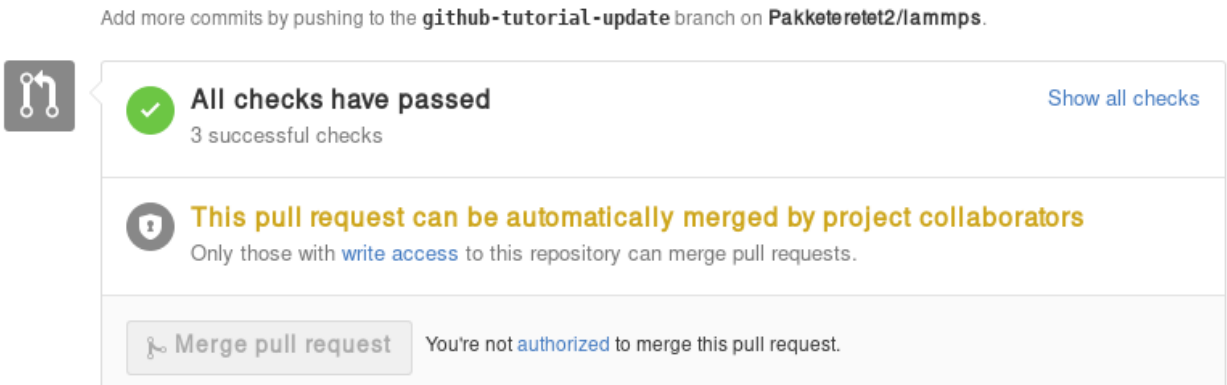
After filing a pull request

Note: When you submit a pull request (or ask for a pull request) for the first time, you will receive an invitation to become a LAMMPS project collaborator. Please accept this invite as being a collaborator will simplify certain administrative tasks and will probably speed up the merging of your feature, too.

You will notice that after filing the pull request, some checks are performed automatically:



If all is fine, you will see this:

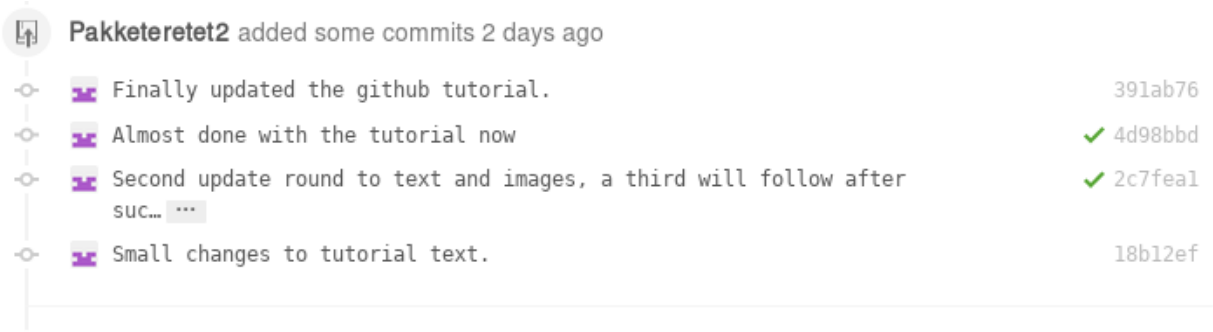


If any of the checks are failing, your pull request will not be processed, as your changes may break compilation for certain configurations or may not merge cleanly. It is your responsibility to remove the reason(s) for the failed test(s). If you need help with this, please contact the LAMMPS developers by adding a comment explaining your problems with resolving the failed tests.

A few further interesting things (can) happen to pull requests before they are included.

Additional changes

First of all, any additional changes you push into your branch in your repository will automatically become part of the pull request:



This means you can add changes that should be part of the feature after filing the pull request, which is useful in case you have forgotten them, or if a developer has requested that something needs to be changed before the feature can be accepted into the official LAMMPS version. After each push, the automated checks are run again.

Labels

LAMMPS developers may add labels to your pull request to assign it to categories (mostly for bookkeeping purposes), but a few of them are important: needs_work, work_in_progress, test-for-regression, and full-regression-test. The first two indicate, that your pull request is not considered to be complete. With "needs_work" the burden is on exclusively on you; while "work_in_progress" can also mean, that a LAMMPS developer may want to add changes. Please watch the comments to the pull requests. The two "test" labels are used to trigger extended tests before the code is merged. This is sometimes done by LAMMPS developers, if they suspect that there may be some subtle side effects from your changes. It is not done by default, because those tests are very time consuming.

Reviews

As of Summer 2018, a pull request needs at least 1 approving review from a LAMMPS developer with write access to the repository. In case your changes touch code that certain developers are associated with, they are auto-requested by the GitHub software. Those associations are set in the file .github/CODEOWNERS Thus if you want to be automatically notified to review when anybody changes files or packages, that you have contributed to LAMMPS, you can add suitable patterns to that file, or a LAMMPS developer may add you.

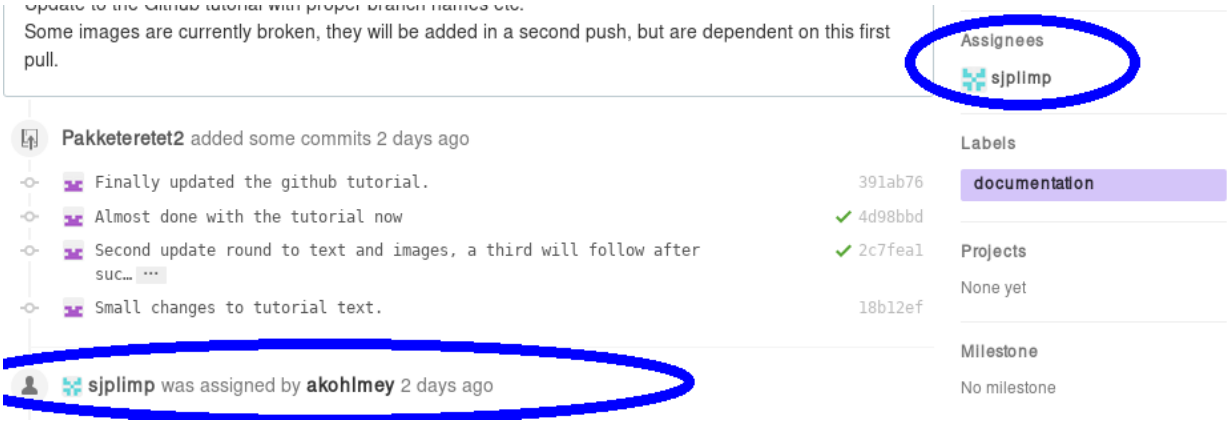
Otherwise, you can also manually request reviews from specific developers, or LAMMPS developers - in their assessment of your pull request - may determine who else should be reviewing your contribution and add that person. Through reviews, LAMMPS developers also may request specific changes from you. If those are not addressed, your pull requests cannot be merged.

Assignees

There is an assignee property for pull requests. If the request has not been reviewed by any developer yet, it is not assigned to anyone. After revision, a developer can choose to assign it to either a) you, b) a LAMMPS developer (including him/herself) or c) Axel Kohlmeyer (akohlmey).

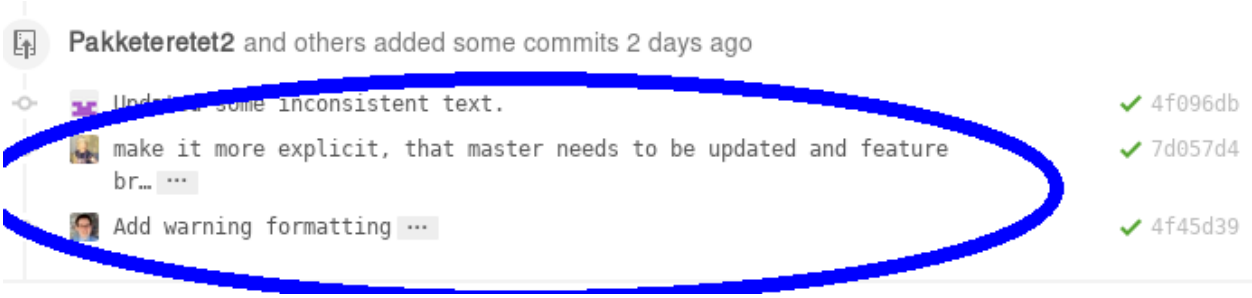
- Case a) happens if changes are required on your part
- Case b) means that at the moment, it is being tested and reviewed by a LAMMPS developer with the expectation that some changes would be required. After the review, the developer can choose to implement changes directly or suggest them to you.
- Case c) means that the pull request has been assigned to the developer overseeing the merging of pull requests into the master branch.

In this case, Axel assigned the tutorial to Steve:



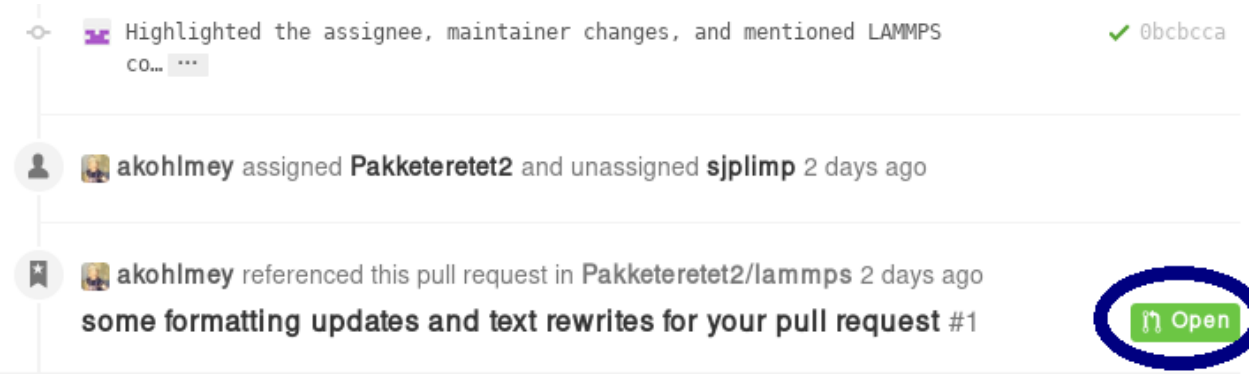
Edits from LAMMPS maintainers

If you allowed edits from maintainers (the default), any LAMMPS maintainer can add changes to your pull request. In this case, both Axel and Richard made changes to the tutorial:

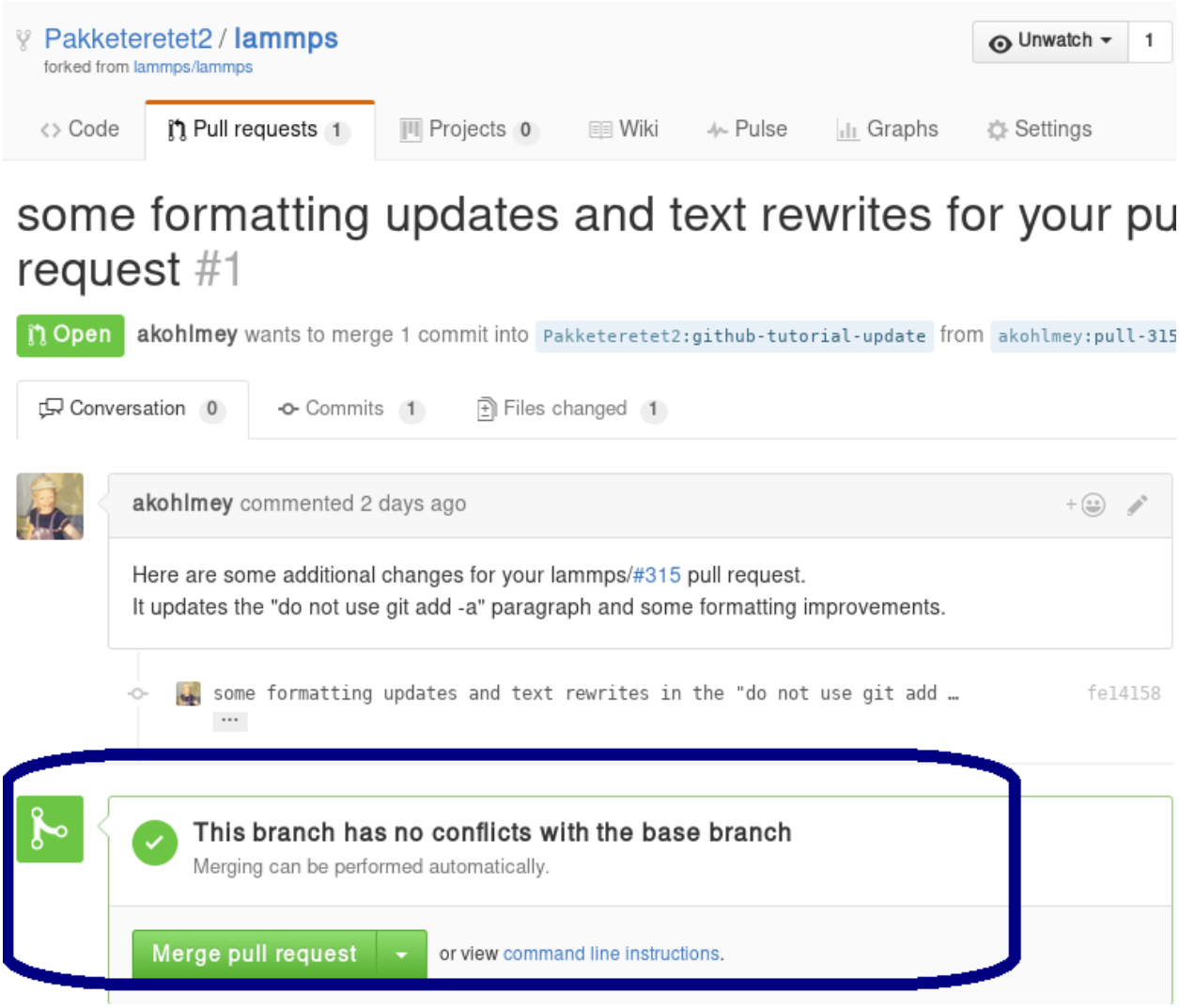


Reverse pull requests

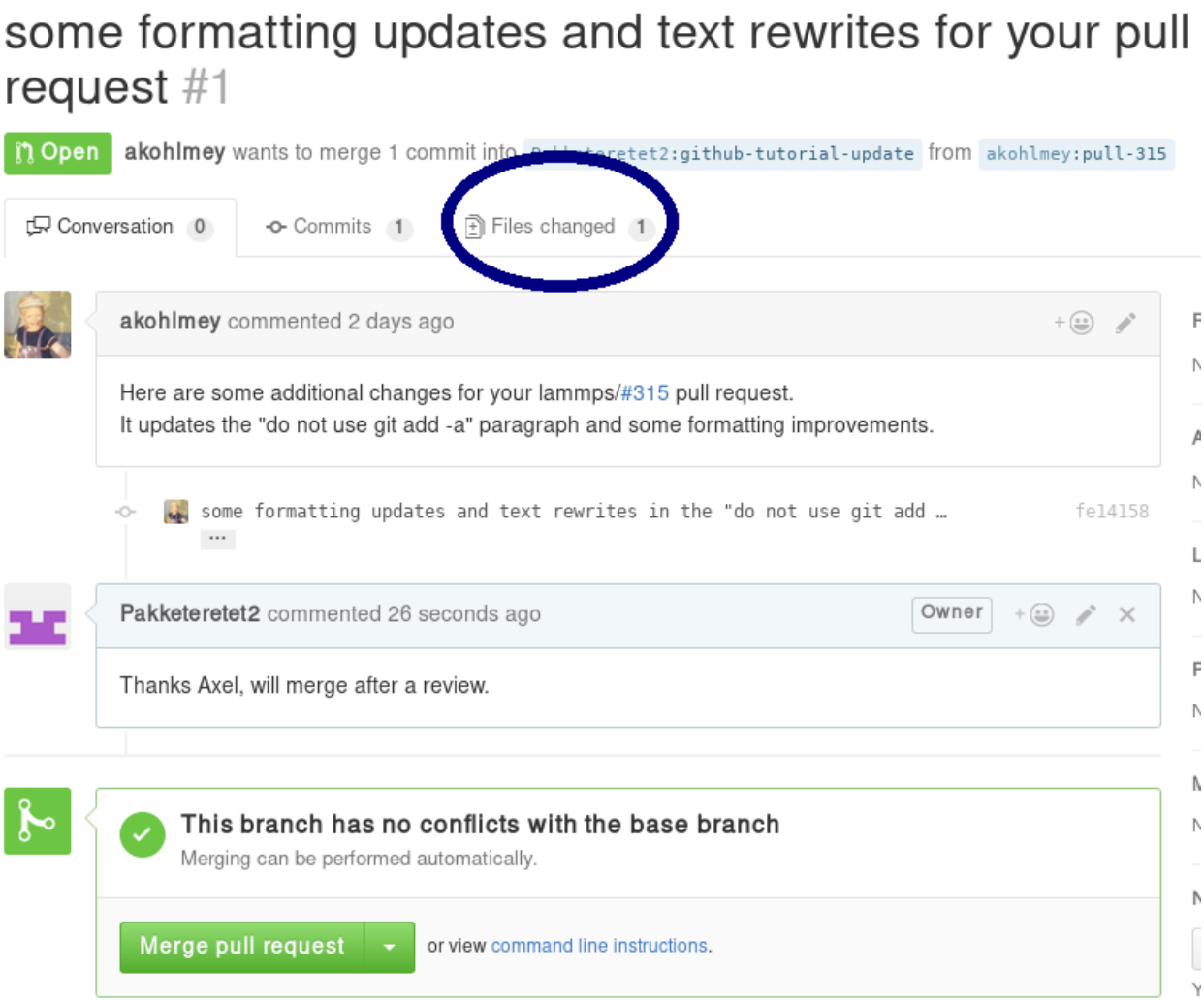
Sometimes, however, you might not feel comfortable having other people push changes into your own branch, or maybe the maintainers are not sure their idea was the right one. In such a case, they can make changes, reassign you as the assignee, and file a "reverse pull request", i.e. file a pull request in your GitHub repository to include changes in the branch, that you have submitted as a pull request yourself. In that case, you can choose to merge their changes back into your branch, possibly make additional changes or corrections and proceed from there. It looks something like this:



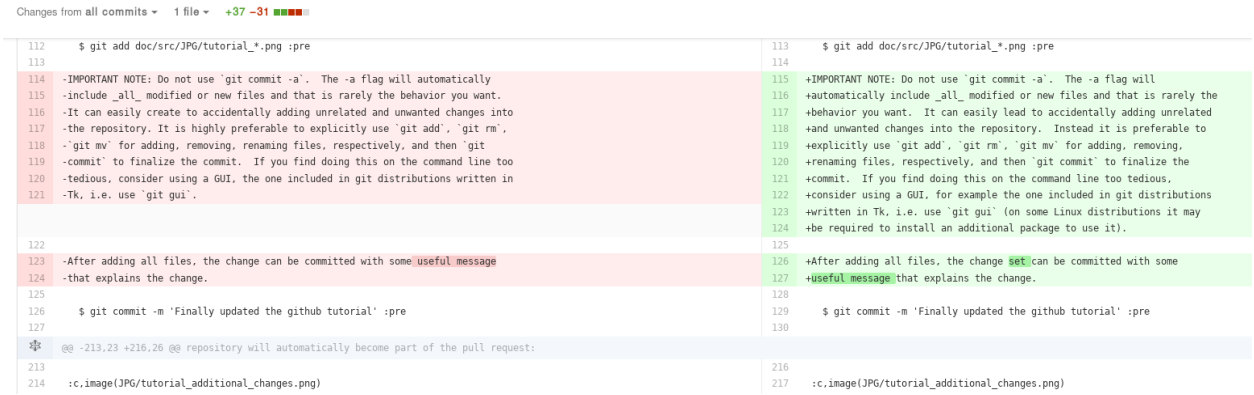
For some reason, the highlighted button didn't work in my case, but I can go to my own repository and merge the pull request from there:



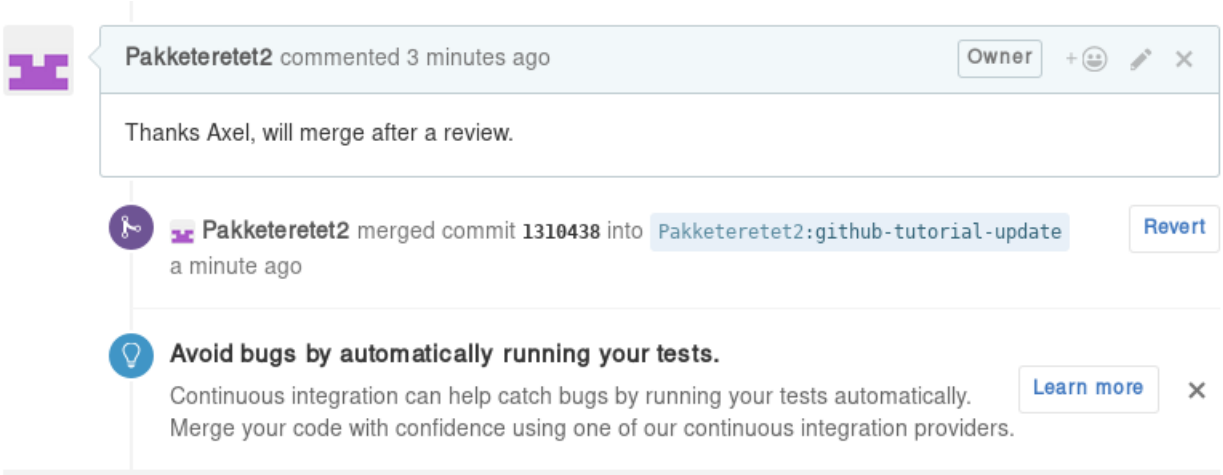
Be sure to check the changes to see if you agree with them by clicking on the tab button:



In this case, most of it is changes in the markup and a short rewrite of Axel's explanation of the "git gui" and "git add" commands.



Because the changes are OK with us, we are going to merge by clicking on "Merge pull request". After a merge it looks like this:



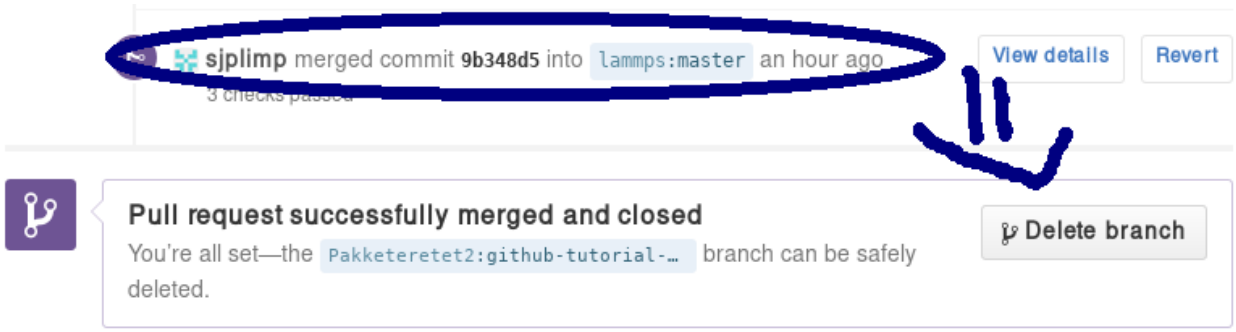
Now, since in the meantime our local text for the tutorial also changed, we need to pull Axel's change back into our branch, and merge them:

```
$ git add Howto_github.txt
$ git add JPG/tutorial_reverse_pull_request*.png
$ git commit -m "Updated text and images on reverse pull requests"
$ git pull
```

In this case, the merge was painless because git could auto-merge:

```
[ stefan@phys8250 src ] % git pull
Auto-merging doc/src/tutorial_github.txt
Waiting for Emacs...
Merge made by the 'recursive' strategy.
 doc/src/tutorial_github.txt | 68 ++++++
```

When everything is fine, the feature branch is merged into the master branch:



Now one question remains: What to do with the feature branch that got merged into upstream?

It is in principle safe to delete them from your own fork. This helps keep it a bit more tidy. Note that you first have to switch to another branch!

```
$ git checkout master
$ git pull master
$ git branch -d github-tutorial-update
```

If you do not pull first, it is not really a problem but git will warn you at the next statement that you are deleting a local branch that was not yet fully merged into HEAD. This is because git does not yet know your branch just got merged into LAMMPS upstream. If you first delete and then pull, everything should still be fine.

Finally, if you delete the branch locally, you might want to push this to your remote(s) as well:

```
$ git push origin :github-tutorial-update
```

Recent changes in the workflow

Some changes to the workflow are not captured in this tutorial. For example, in addition to the master branch, to which all new features should be submitted, there is now also an "unstable" and a "stable" branch; these have the same content as "master", but are only updated after a patch release or stable release was made. Furthermore, the naming of the patches now follow the pattern "patch_<Day><Month><Year>" to simplify comparisons between releases. Finally, all patches and submissions are subject to automatic testing and code checks to make sure they at the very least compile.

A discussion of the LAMMPS developer GitHub workflow can be found in the file doc/github-development-workflow.md

8.1.2 PyLammps Tutorial

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    - *Comparison of lammps and PyLammps interfaces*
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    * *Installation inside of a virtualenv*
        · *Benefits of using a virtualenv*
        · *Creating a virtualenv with lammps installed*
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    * *Running a Monte Carlo relaxation*
  - *Using PyLammps and mpi4py (Experimental)*
  - *Feedback and Contributing*

Overview

PyLammps is a Python wrapper class which can be created on its own or use an existing lammps Python object. It creates a simpler, Python-like interface to common LAMMPS functionality, in contrast to the lammps.py wrapper on the C-style LAMMPS library interface which is written using Python ctypes. The lammps.py wrapper is discussed on the *Python library* doc page.

Unlike the flat ctypes interface, PyLammps exposes a discoverable API. It no longer requires knowledge of the underlying C++ code implementation. Finally, the IPyLammps wrapper builds on top of PyLammps and adds some additional features for IPython integration into IPython notebooks, e.g. for embedded visualization output from dump/image.

Comparison of lammps and PyLammps interfaces

lammps.lammps

- uses C-Types
- direct memory access to native C++ data
- provides functions to send and receive data to LAMMPS
- requires knowledge of how LAMMPS internally works (C pointers, etc)

lammps.PyLammps

- higher-level abstraction built on top of original C-Types interface
- manipulation of Python objects
- communication with LAMMPS is hidden from API user
- shorter, more concise Python
- better IPython integration, designed for quick prototyping

Quick Start

System-wide Installation

Step 1: Building LAMMPS as a shared library

To use LAMMPS inside of Python it has to be compiled as shared library. This library is then loaded by the Python interface. In this example we enable the MOLECULE package and compile LAMMPS with C++ exceptions, PNG, JPEG and FFMPEG output support enabled.

Step 1a: For the CMake based build system, the steps are:

```
mkdir $LAMMPS_DIR/build-shared
cd  $LAMMPS_DIR/build-shared

# MPI, PNG, Jpeg, FFMPEG are auto-detected
cmake ../cmake -DPKG_MOLECULE=yes -DLAMMPS_EXCEPTIONS=yes -DBUILD_LIB=yes -DBUILD_
↪SHARED_LIBS=yes
make
```

Step 1b: For the legacy, make based build system, the steps are:

```
cd $LAMMPS_DIR/src

# add packages if necessary
make yes-MOLECULE

# compile shared library using Makefile
make mpi mode=shlib LMP_INC="-DLAMMPS_PNG -DLAMMPS_JPEG -DLAMMPS_FFMPEG -DLAMMPS_
↪EXCEPTIONS" JPG_LIB="-lpng -ljpeg"
```

Step 2: Installing the LAMMPS Python package

PyLammps is part of the lammps Python package. To install it simply install that package into your current Python installation with:

```
make install-python
```

Note: Recompiling the shared library requires re-installing the Python package

Installation inside of a virtualenv

You can use virtualenv to create a custom Python environment specifically tuned for your workflow.

Benefits of using a virtualenv

- isolation of your system Python installation from your development installation
- installation can happen in your user directory without root access (useful for HPC clusters)
- installing packages through pip allows you to get newer versions of packages than e.g., through apt-get or yum package managers (and without root access)
- you can even install specific old versions of a package if necessary

Prerequisite (e.g. on Ubuntu)

```
apt-get install python-virtualenv
```

Creating a virtualenv with lammps installed

```
# create virtualenv named 'testing'
virtualenv $HOME/python/testing

# activate 'testing' environment
source $HOME/python/testing/bin/activate
```

Now configure and compile the LAMMPS shared library as outlined above. When using CMake and the shared library has already been build, you need to re-run CMake to update the location of the python executable to the location in the virtual environment with:

```
cmake . -DPYTHON_EXECUTABLE=$(which python)

# install LAMMPS package in virtualenv
(testing) make install-python

# install other useful packages
(testing) pip install matplotlib jupyter mpi4py

...

# return to original shell
(testing) deactivate
```

Creating a new instance of PyLammps

To create a PyLammps object you need to first import the class from the lammps module. By using the default constructor, a new *lammps* instance is created.

```
from lammps import PyLammps
L = PyLammps()
```

You can also initialize PyLammps on top of this existing *lammps* object:

```
from lammps import lammps, PyLammps
lmp = lammps()
L = PyLammps(ptr=lmp)
```

Commands

Sending a LAMMPS command with the existing library interfaces is done using the command method of the lammps object instance.

For instance, let's take the following LAMMPS command:

```
region box block 0 10 0 5 -0.5 0.5
```

In the original interface this command can be executed with the following Python code if *L* was a lammps instance:

```
L.command("region box block 0 10 0 5 -0.5 0.5")
```

With the PyLammps interface, any command can be split up into arbitrary parts separated by white-space, passed as individual arguments to a region method.

```
L.region("box block", 0, 10, 0, 5, -0.5, 0.5)
```

Note that each parameter is set as Python literal floating-point number. In the PyLammps interface, each command takes an arbitrary parameter list and transparently merges it to a single command string, separating individual parameters by white-space.

The benefit of this approach is avoiding redundant command calls and easier parameterization. In the original interface parameterization needed to be done manually by creating formatted strings.

```
L.command("region box block %f %f %f %f %f %f" % (xlo, xhi, ylo, yhi, zlo, zhi))
```

In contrast, methods of PyLammps accept parameters directly and will convert them automatically to a final command string.

```
L.region("box block", xlo, xhi, ylo, yhi, zlo, zhi)
```

System state

In addition to dispatching commands directly through the PyLammps object, it also provides several properties which allow you to query the system state.

L.system Is a dictionary describing the system such as the bounding box or number of atoms

L.system.xlo, L.system.xhi bounding box limits along x-axis

L.system.ylo, L.system.yhi bounding box limits along y-axis

L.system.zlo, L.system.zhi bounding box limits along z-axis

L.communication configuration of communication subsystem, such as the number of threads or processors

L.communication.nthreads number of threads used by each LAMMPS process

L.communication.nprocs number of MPI processes used by LAMMPS

L.fixes List of fixes in the current system

L.computes List of active computes in the current system

L.dump List of active dumps in the current system

L.groups List of groups present in the current system

Working with LAMMPS variables

LAMMPS variables can be both defined and accessed via the PyLammps interface.

To define a variable you can use the *variable* command:

```
L.variable("a index 2")
```

A dictionary of all variables is returned by L.variables

you can access an individual variable by retrieving a variable object from the L.variables dictionary by name

```
a = L.variables['a']
```

The variable value can then be easily read and written by accessing the value property of this object.

```
print(a.value)
a.value = 4
```

Retrieving the value of an arbitrary LAMMPS expressions

LAMMPS expressions can be immediately evaluated by using the eval method. The passed string parameter can be any expression containing global thermo values, variables, compute or fix data.

```
result = L.eval("ke") # kinetic energy
result = L.eval("pe") # potential energy

result = L.eval("v_t/2.0")
```

Accessing atom data

All atoms in the current simulation can be accessed by using the L.atoms list. Each element of this list is an object which exposes its properties (id, type, position, velocity, force, etc.).

```
# access first atom
L.atoms[0].id
L.atoms[0].type

# access second atom
L.atoms[1].position
L.atoms[1].velocity
L.atoms[1].force
```

Some properties can also be used to set:

```
# set position in 2D simulation
L.atoms[0].position = (1.0, 0.0)

# set position in 3D simulation
L.atoms[0].position = (1.0, 0.0, 1.)
```

Evaluating thermo data

Each simulation run usually produces thermo output based on system state, computes, fixes or variables. The trajectories of these values can be queried after a run via the L.runs list. This list contains a growing list of run data. The first element is the output of the first run, the second element that of the second run.

```
L.run(1000)
L.runs[0] # data of first 1000 time steps

L.run(1000)
L.runs[1] # data of second 1000 time steps
```

Each run contains a dictionary of all trajectories. Each trajectory is accessible through its thermo name:

```
L.runs[0].thermo.Step # list of time steps in first run
L.runs[0].thermo.Ke   # list of kinetic energy values in first run
```

Together with matplotlib plotting data out of LAMMPS becomes simple:

```
import matplotlib.plot as plt
steps = L.runs[0].thermo.Step
ke    = L.runs[0].thermo.Ke
plt.plot(steps, ke)
```

Error handling with PyLammps

Compiling the shared library with C++ exception support provides a better error handling experience. Without exceptions the LAMMPS code will terminate the current Python process with an error message. C++ exceptions allow capturing them on the C++ side and rethrowing them on the Python side. This way you can handle LAMMPS errors through the Python exception handling mechanism.

> **Warning:** Capturing a LAMMPS exception in Python can still mean that the current LAMMPS process is in an illegal state and must be terminated. It is advised to save your data and terminate the Python instance as quickly as possible.

Using PyLammps in IPython notebooks and Jupyter

If the LAMMPS Python package is installed for the same Python interpreter as IPython, you can use PyLammps directly inside of an IPython notebook inside of Jupyter. Jupyter is a powerful integrated development environment (IDE) for many dynamic languages like Python, Julia and others, which operates inside of any web browser. Besides auto-completion and syntax highlighting it allows you to create formatted documents using Markup, mathematical formulas, graphics and animations intermixed with executable Python code. It is a great format for tutorials and showcasing your latest research.

To launch an instance of Jupyter simply run the following command inside your Python environment (this assumes you followed the Quick Start instructions):

```
jupyter notebook
```

IPyLammps Examples

Examples of IPython notebooks can be found in the python/examples/pylammps sub-directory. To open these notebooks launch *jupyter notebook* inside this directory and navigate to one of them. If you compiled and installed a LAMMPS shared library with exceptions, PNG, JPEG and FFMPEG support you should be able to rerun all of these notebooks.

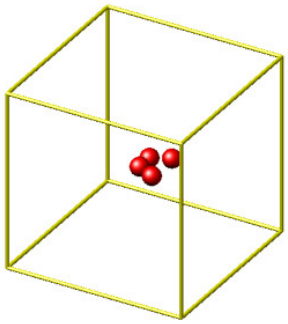
Validating a dihedral potential

This example showcases how an IPython Notebook can be used to compare a simple LAMMPS simulation of a harmonic dihedral potential to its analytical solution. Four atoms are placed in the simulation and the dihedral potential is applied on them using a datafile. Then one of the atoms is rotated along the central axis by setting its position from Python, which changes the dihedral angle.

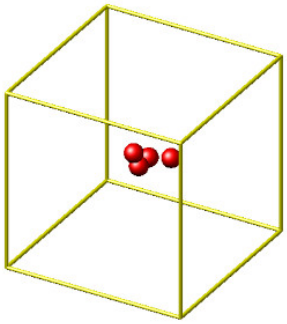
```
phi = [d \* math.pi / 180 for d in range(360)]

pos = [(1.0, math.cos(p), math.sin(p)) for p in phi]

pe = []
for p in pos:
    L.atoms[3].position = p
    L.run(0)
    pe.append(L.eval("pe"))
```

By evaluating the potential energy for each position we can verify that trajectory with the analytical formula. To compare both solutions, we plot both trajectories over each other using matplotlib, which embeds the generated plot inside the IPython notebook.

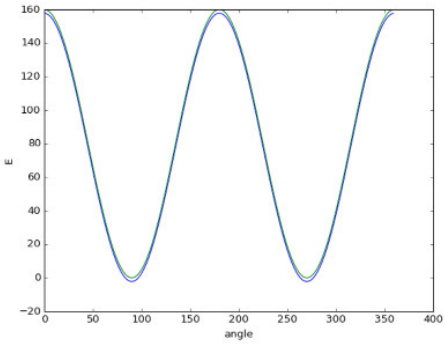
```
In [11]: L.image(zoom=1.0)
Out[11]:
```



```
In [14]: L.image(zoom=1.0)
Out[14]:
```



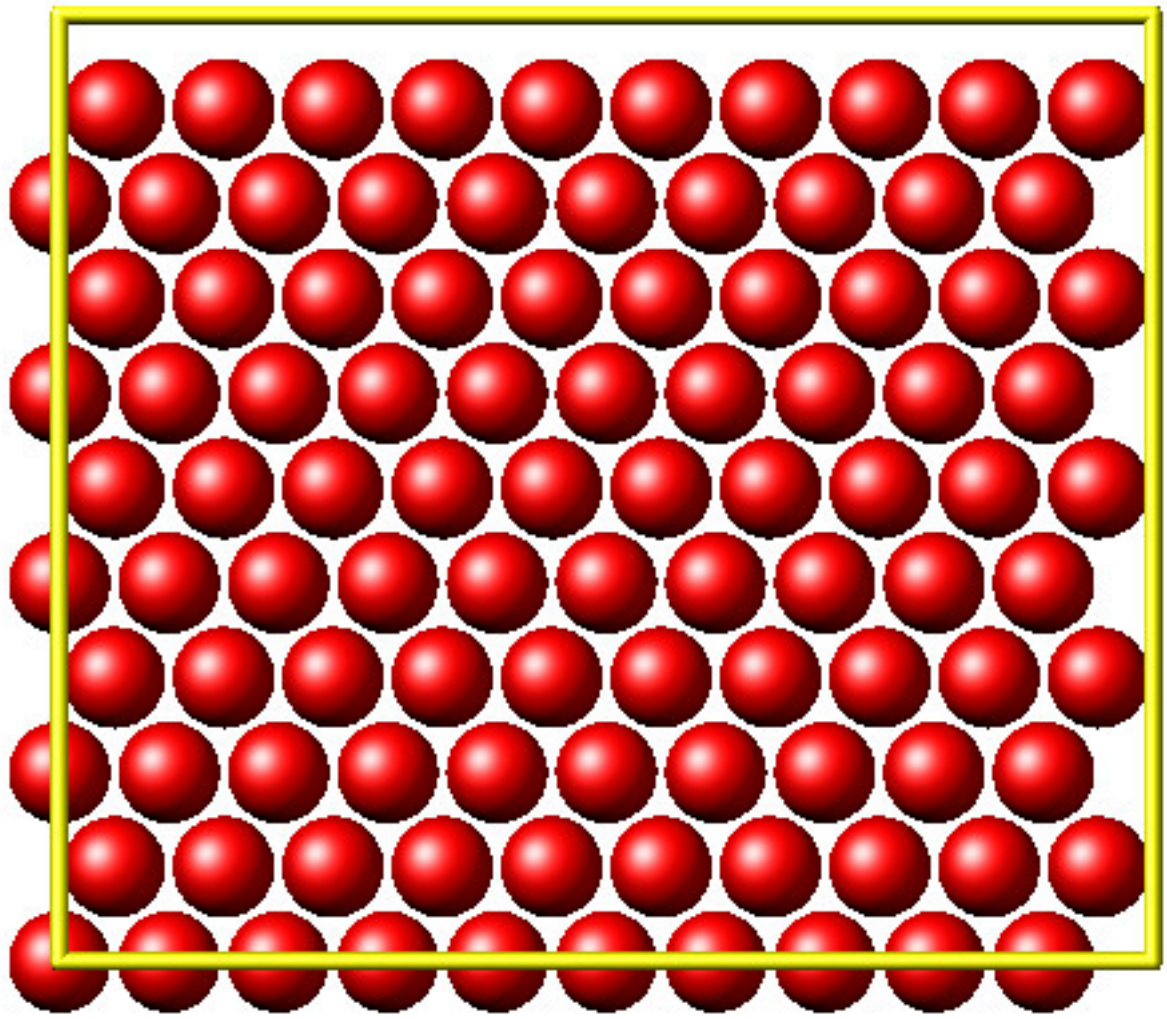
```
In [27]: plt.plot(range(360), pe, range(360), E_analytical)
         plt.xlabel('angle')
         plt.ylabel('E')
```



Running a Monte Carlo relaxation

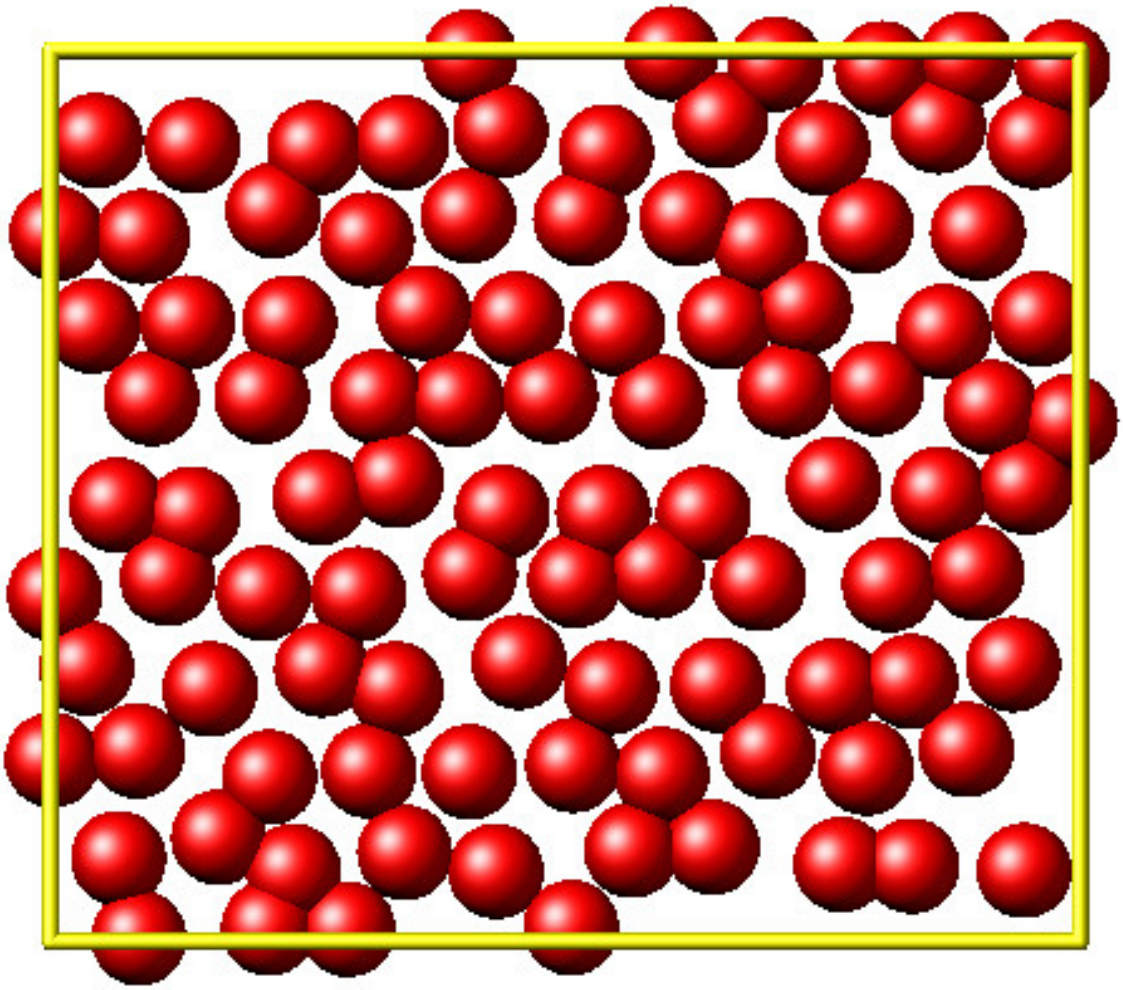
This second example shows how to use PyLammps to create a 2D Monte Carlo Relaxation simulation, computing and plotting energy terms and even embedding video output.

Initially, a 2D system is created in a state with minimal energy.



It is then disordered by moving each atom by a random delta.

```
random.seed(27848)
deltaperturb = 0.2

for i in range(L.system.natoms):
    x, y = L.atoms[i].position
    dx = deltaperturb \* random.uniform(-1, 1)
    dy = deltaperturb \* random.uniform(-1, 1)
    L.atoms[i].position  = (x+dx, y+dy)

L.run(0)
```



Finally, the Monte Carlo algorithm is implemented in Python. It continuously moves random atoms by a random delta and only accepts certain moves.

```
estart = L.eval("pe")
elast = estart

naccept = 0
energies = [estart]

niterations = 3000
deltamove = 0.1
kT = 0.05

natoms = L.system.natoms

for i in range(niterations):
    iatom = random.randrange(0, natoms)
    current_atom = L.atoms[iatom]

    x0, y0 = current_atom.position
```

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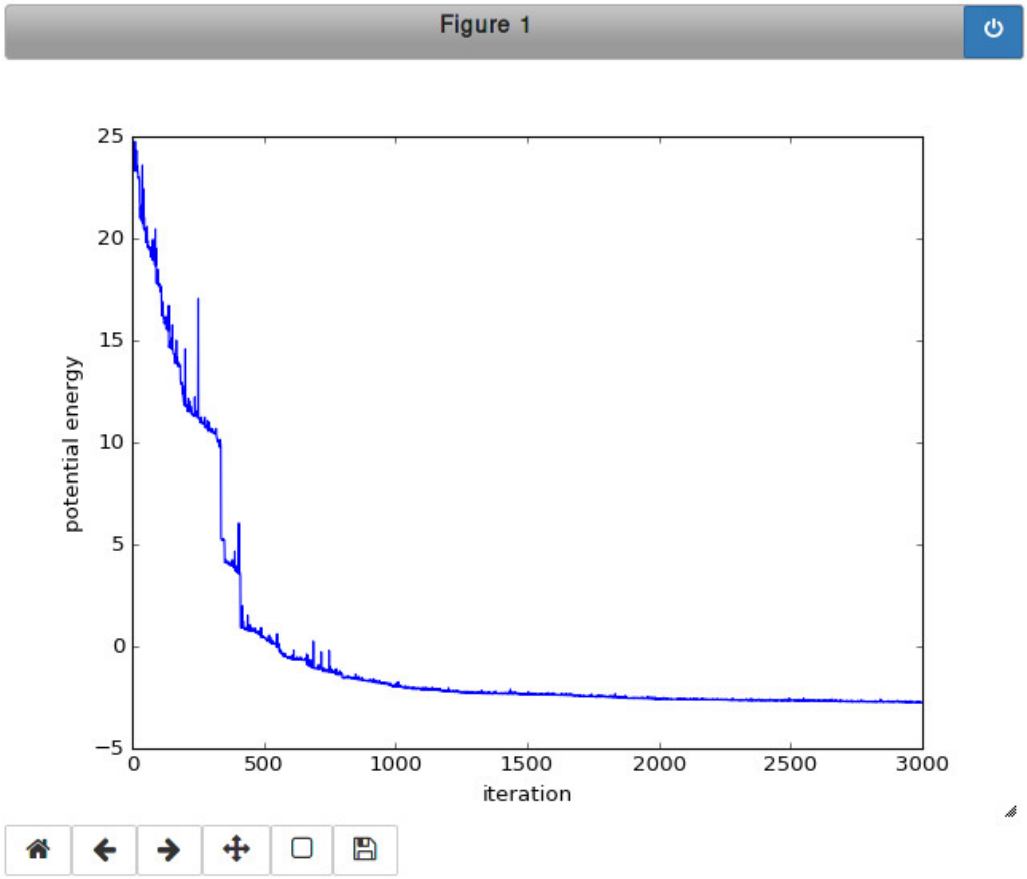
```
    dx = deltamove \* random.uniform(-1, 1)
    dy = deltamove \* random.uniform(-1, 1)

    current_atom.position = (x0+dx, y0+dy)

    L.run(1, "pre no post no")

    e = L.eval("pe")
    energies.append(e)

    if e <= elast:
        naccept += 1
        elast = e
    elif random.random() <= math.exp(natoms\*(elast-e)/kT):
        naccept += 1
        elast = e
    else:
        current_atom.position = (x0, y0)
```

The energies of each iteration are collected in a Python list and finally plotted using matplotlib.

```
In [20]: plt.xlabel('iteration')
         plt.ylabel('potential energy')
         plt.plot(energies)
```




```
Out[20]: [<matplotlib.lines.Line2D at 0x7f26a40123c8>]
```

The IPython notebook also shows how to use dump commands and embed video files inside of the IPython notebook.

Using PyLammps and mpi4py (Experimental)

PyLammps can be run in parallel using mpi4py. This python package can be installed using

```
pip install mpi4py
```

The following is a short example which reads in an existing LAMMPS input file and executes it in parallel. You can find in.melt in the examples/melt folder.

```
from mpi4py import MPI
from lammps import PyLammps

L = PyLammps()
L.file("in.melt")

if MPI.COMM_WORLD.rank == 0:
    print("Potential energy: ", L.eval("pe"))
```

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```
MPI.Finalize()
```

To run this script (melt.py) in parallel using 4 MPI processes we invoke the following mpirun command:

```
mpirun -np 4 python melt.py
```

Warning: Any command must be executed by all MPI processes. However, evaluations and querying the system state is only available on rank 0.

Feedback and Contributing

If you find this Python interface useful, please feel free to provide feedback and ideas on how to improve it to Richard Berger (richard.berger@temple.edu). We also want to encourage people to write tutorial style IPython notebooks showcasing LAMMPS usage and maybe their latest research results.

8.1.3 Using LAMMPS with Bash on Windows

written by Richard Berger

Starting with Windows 10 you can install Linux tools directly in Windows. This allows you to compile LAMMPS following the same procedure as on a real Ubuntu Linux installation. Software can be easily installed using the package manager via apt-get and all files are accessible in both the Windows Explorer and your Linux shell (bash). This avoids switching to a different operating system or installing a virtual machine. Everything runs on Windows.

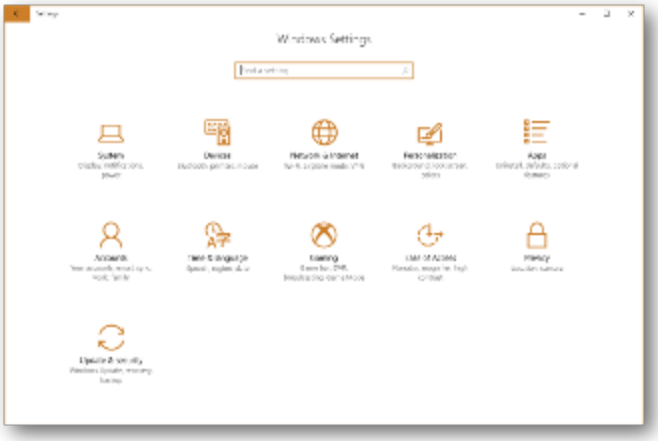
Installing Bash on Windows

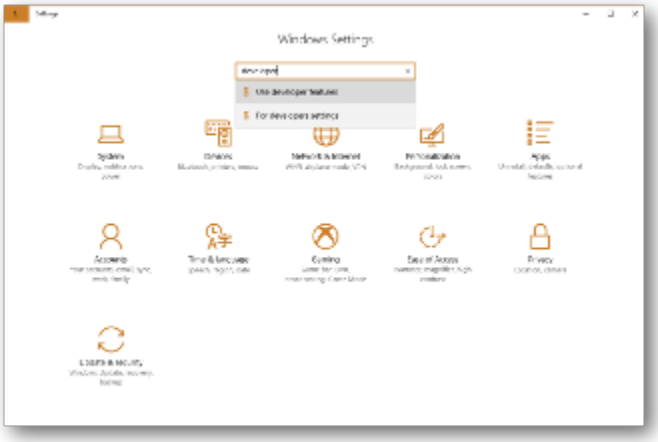
Prerequisites

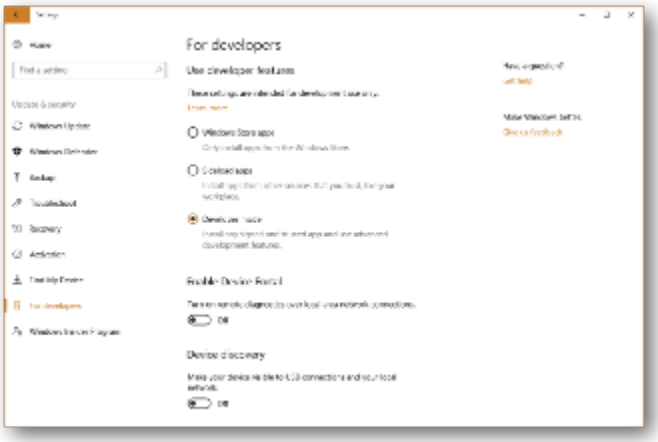
- Windows 10 (64bit only)
- Latest updates installed

Enable developer mode

You enable this feature by first opening Windows Settings and enabling Developer mode. Go to the Windows settings and search for "developer". This will allow you to install software which comes from outside of the Windows Store. You might be prompted to reboot your compute. Please do so.

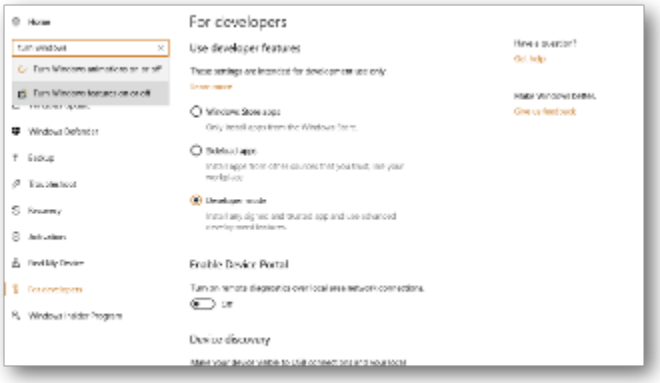


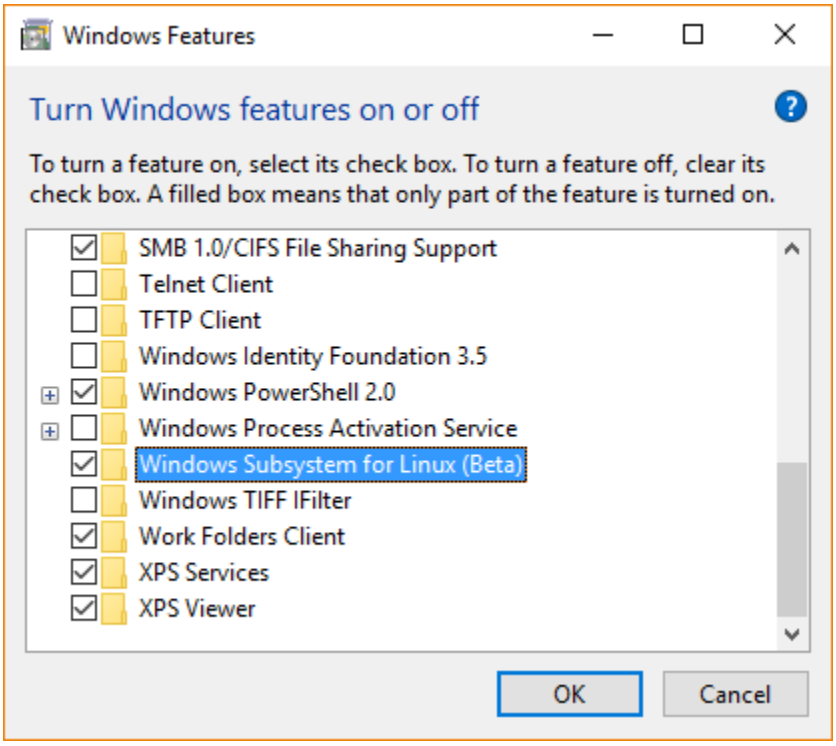




Install Windows Subsystem for Linux

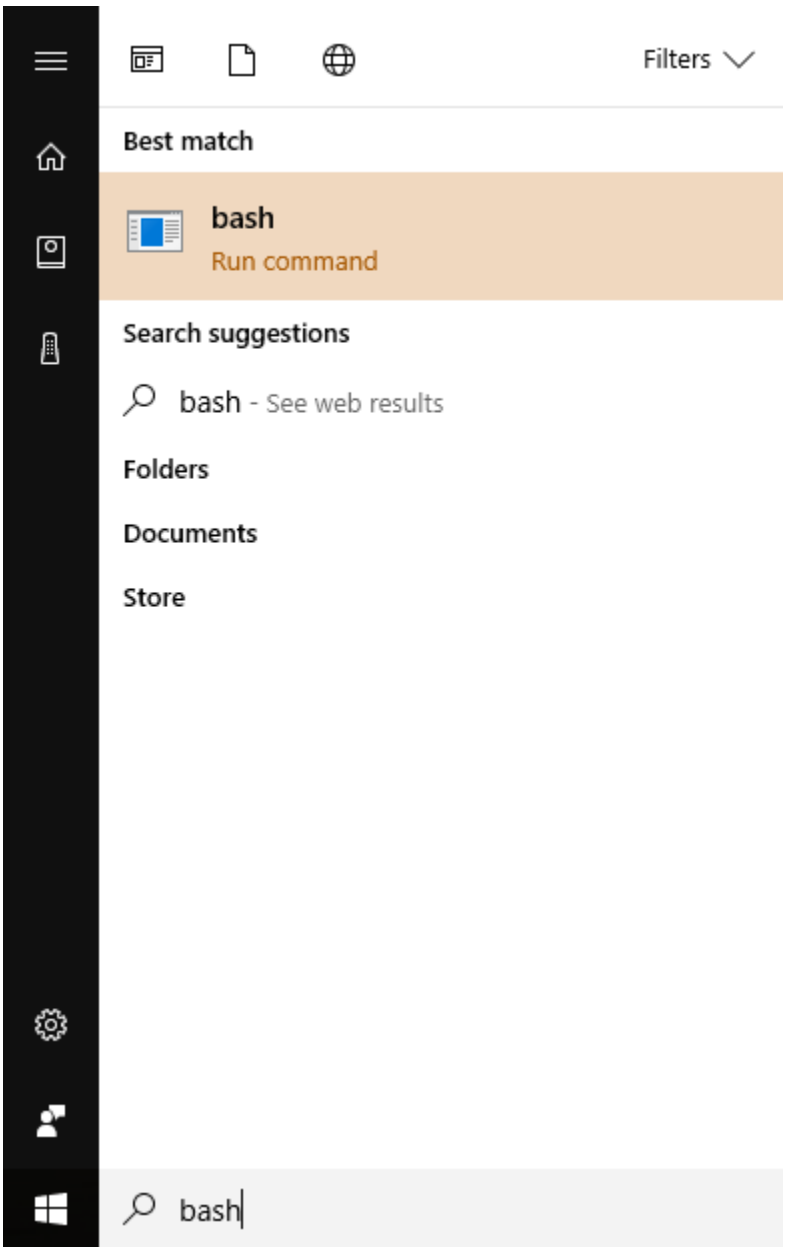
Next you must ensure that the Window Subsystem for Linux is installed. Again, search for "enable windows features" in the Settings dialog. This opens a dialog with a list of features you can install. Add a checkmark to Windows Subsystem for Linux (Beta) and press OK.

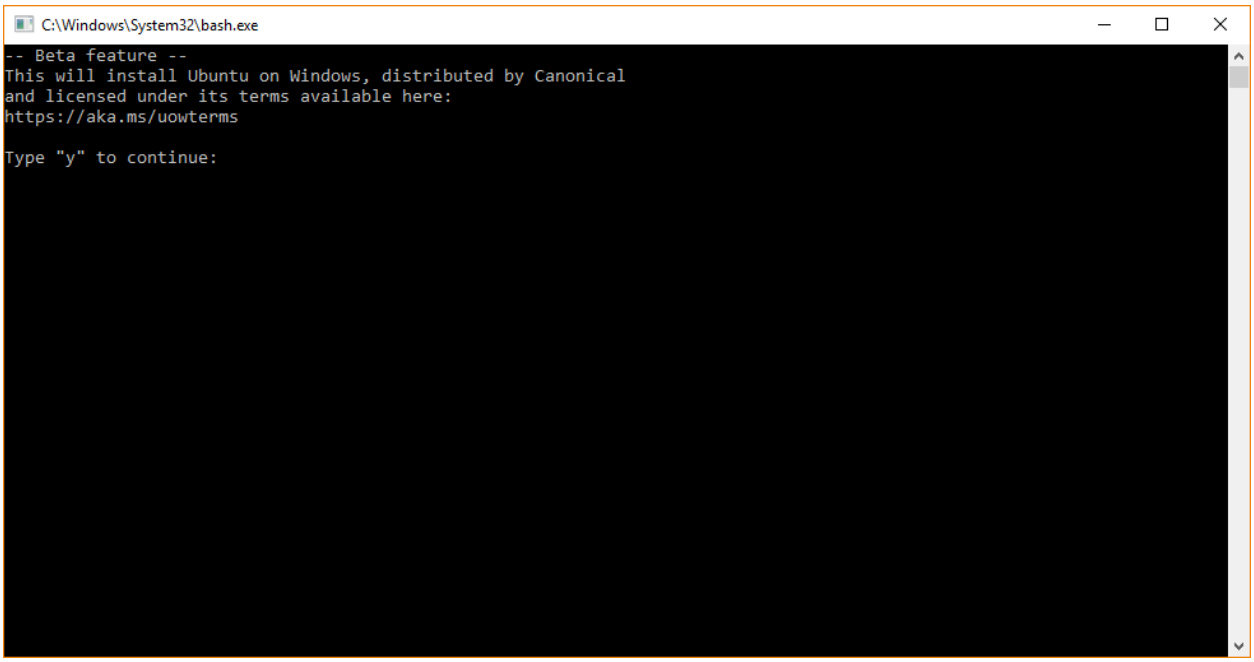




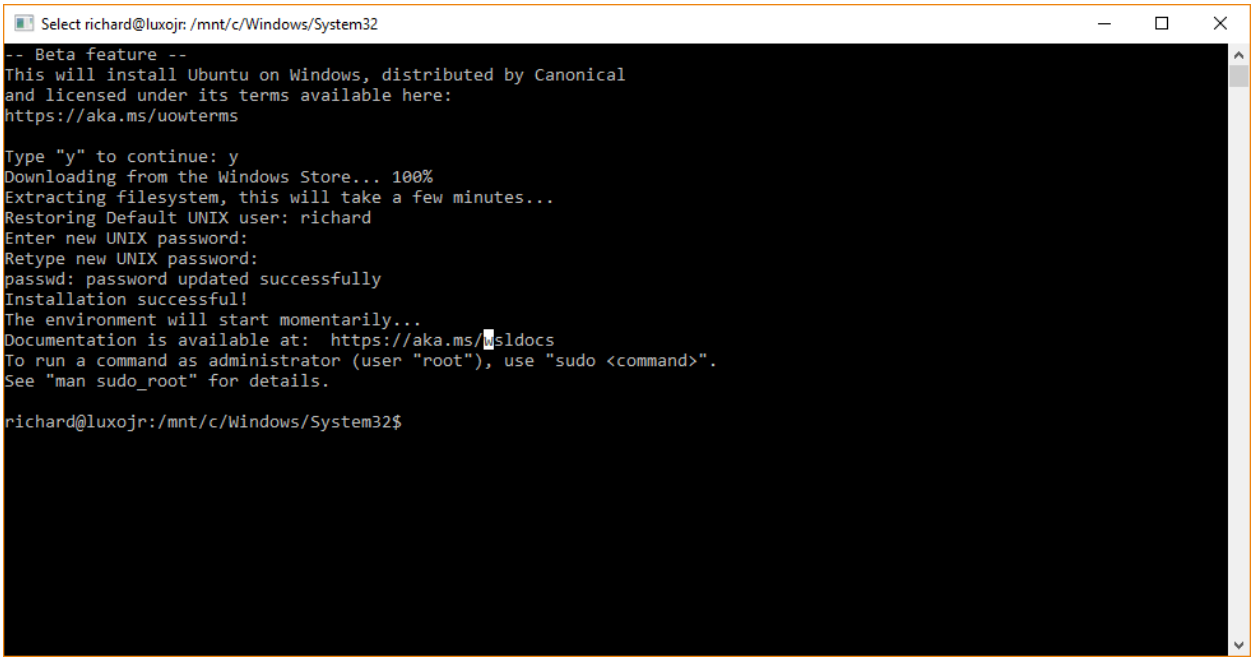
Install Bash for Windows

After installation completes, type "bash" in the Windows Start menu search. Select the first found option. This will launch a command-line window which will prompt you about installing Ubuntu on Windows. Confirm with "y" and press enter. This will then download Ubuntu for Windows.



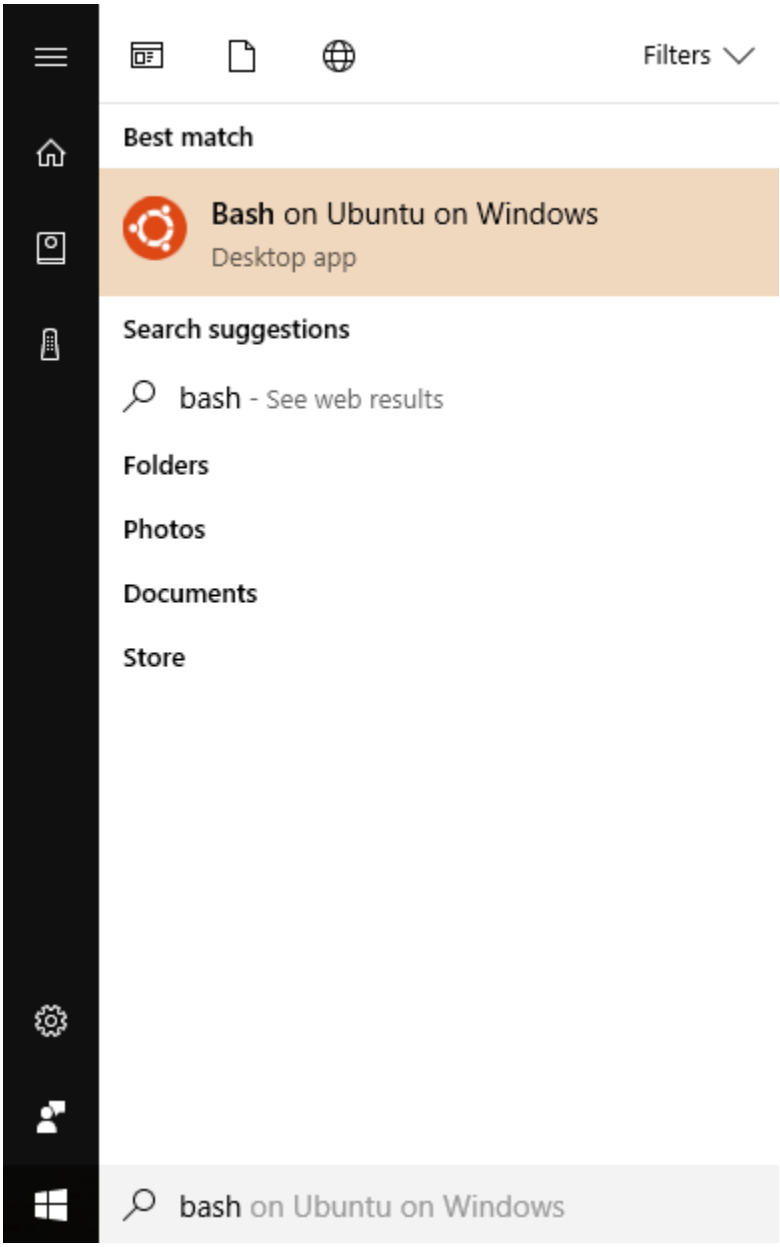


During installation, you will be asked for a new password. This will be used for installing new software and running commands with sudo.

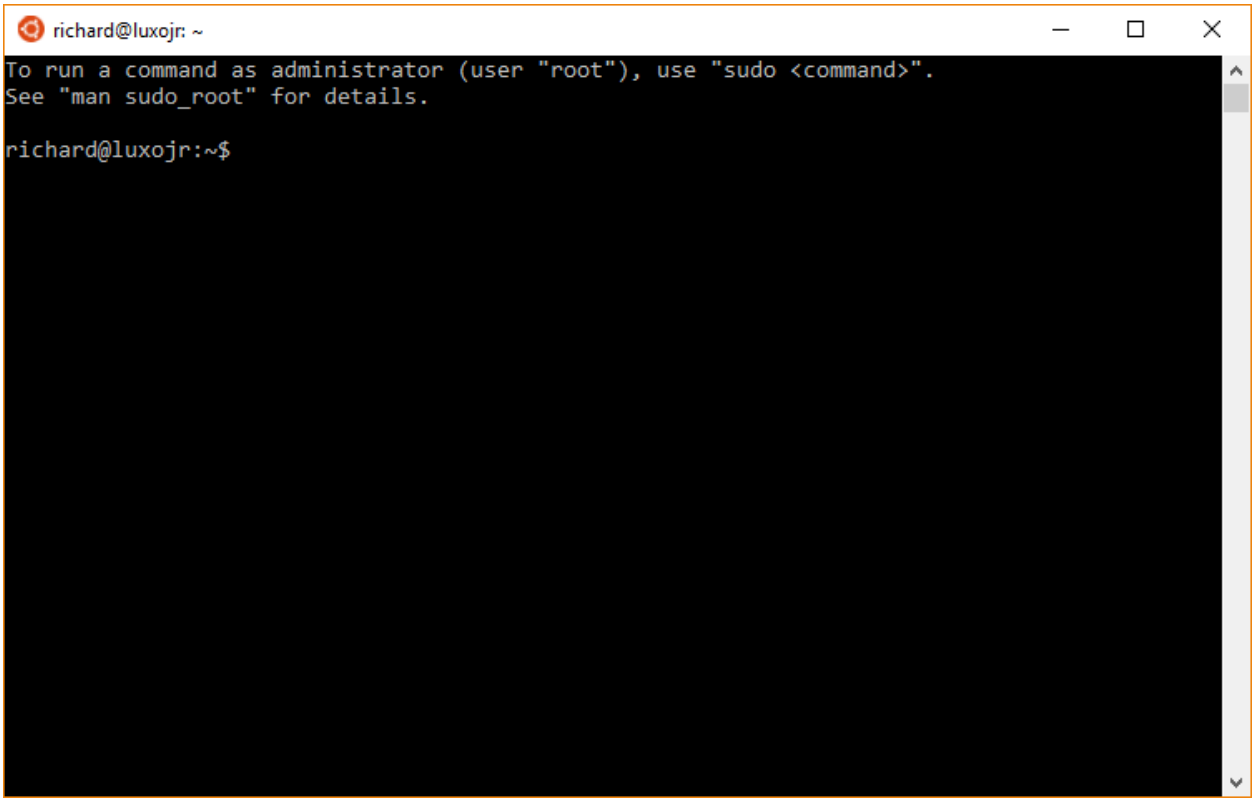


Type exit to close the command-line window.

Go to the Start menu and type “bash” again. This time you will see a “Bash on Ubuntu on Windows” Icon. Start this program.



Congratulations, you have installed **Bash on Ubuntu on Windows**.



Compiling LAMMPS in Bash on Windows

The installation of LAMMPS in this environment is identical to working inside of a real Ubuntu Linux installation. At the time writing, it uses Ubuntu 16.04.

Installing prerequisite packages

First upgrade all existing packages using

```
sudo apt update
sudo apt upgrade -y
```

Next install the following packages, which include compilers and libraries needed for various LAMMPS features:

```
sudo apt install -y build-essential ccache gfortran openmpi-bin libopenmpi-dev␣
↪libfftw3-dev libjpeg-dev libpng12-dev python-dev python-virtualenv libblas-dev␣
↪liblapack-dev libhdf5-serial-dev hdf5-tools
```

Files in Ubuntu on Windows

When you launch "Bash on Ubuntu on Windows" you will start out in your Linux user home directory /home/[username]. You can access your Windows user directory using the /mnt/c/Users/[username] folder.

Download LAMMPS

Obtain a copy of the LAMMPS code and go into it using "cd"

Option 1: Downloading LAMMPS tarball using wget

```
wget http://lammps.sandia.gov/tars/lammps-stable.tar.gz
tar xvzf lammps-stable.tar.gz
cd lammps-31Mar17
```

Option 2: Obtaining LAMMPS code from GitHub

```
git clone https://github.com/lammps/lammps.git
cd lammps
```

Compiling LAMMPS

At this point you can compile LAMMPS like on Ubuntu Linux.

Compiling serial version

```
cd src/
make -j 4 serial
```

This will create an executable called lmp_serial in the src/ directory

Compiling MPI version

```
cd src/
make -j 4 mpi
```

This will create an executable called lmp_mpi in the src/ directory

---

Finally, please note the absolute path of your src folder. You can get this using

```
pwd
```

or

```
echo $PWD
```

To run any examples you need the location of the executable. For now, let us save this location in a temporary variable

```
LAMMPS_DIR=$PWD
```

Running an example script

Once compiled you can execute some of the LAMMPS examples. Switch into the examples/melt folder

```
cd ../examples/melt
```

The full path of the serial executable is $LAMMPS_DIR/lmp_serial, while the mpi version is $LAMMPS_DIR/lmp_mpi. You can run the melt example with either version as follows:

```
$LAMMPS_DIR/lmp_serial -in in.melt
```

or

```
mpirun -np 4 $LAMMPS_DIR/lmp_mpi -in in.melt
```

Note the use of our variable $LAMMPS_DIR, which expands into the full path of the LAMMPS src folder we saved earlier.

Adding your executable directory to your PATH

You can avoid having to type the full path of your LAMMPS binary by adding its parent folder to the PATH environment variable as follows:

```
export PATH=$LAMMPS_DIR:$PATH
```

Input scripts can then be run like this:

```
lmp_serial -in in.melt
```

or

```
mpirun -np 4 lmp_mpi -in in.melt
```

However, this PATH variable will not persist if you close your bash window. To persist this setting edit the $HOME/.bashrc file using your favorite editor and add this line

```
export PATH=/full/path/to/your/lammps/src:$PATH
```

Example:

For an executable lmp_serial with a full path

```
/home/richard/lammps/src/lmp_serial
```

the PATH variable should be

```
export PATH=/home/richard/lammps/src:$PATH
```

Note: This should give you a jump start when trying to run LAMMPS on Windows. To become effective in this environment I encourage you to look into Linux tutorials explaining Bash and Basic Unix commands (e.g., Linux Journey)

8.2 General howto

8.2.1 Restart a simulation

There are 3 ways to continue a long LAMMPS simulation. Multiple *run* commands can be used in the same input script. Each run will continue from where the previous run left off. Or binary restart files can be saved to disk using the *restart* command. At a later time, these binary files can be read via a *read_restart* command in a new script. Or they can be converted to text data files using the *-r command-line switch* and read by a *read_data* command in a new script.

Here we give examples of 2 scripts that read either a binary restart file or a converted data file and then issue a new run command to continue where the previous run left off. They illustrate what settings must be made in the new script. Details are discussed in the documentation for the *read_restart* and *read_data* commands.

Look at the *in.chain* input script provided in the *bench* directory of the LAMMPS distribution to see the original script that these 2 scripts are based on. If that script had the line

```
restart         50 tmp.restart
```

added to it, it would produce 2 binary restart files (tmp.restart.50 and tmp.restart.100) as it ran.

This script could be used to read the 1st restart file and re-run the last 50 timesteps:

```
read_restart    tmp.restart.50

neighbor        0.4 bin
neigh_modify    every 1 delay 1

fix             1 all nve
fix             2 all langevin 1.0 1.0 10.0 904297

timestep        0.012

run             50
```

Note that the following commands do not need to be repeated because their settings are included in the restart file: *units, atom_style, special_bonds, pair_style, bond_style*. However these commands do need to be used, since their settings are not in the restart file: *neighbor, fix, timestep*.

If you actually use this script to perform a restarted run, you will notice that the thermodynamic data match at step 50 (if you also put a "thermo 50" command in the original script), but do not match at step 100. This is because the *fix langevin* command uses random numbers in a way that does not allow for perfect restarts.

As an alternate approach, the restart file could be converted to a data file as follows:

```
lmp_g++ -r tmp.restart.50 tmp.restart.data
```

Then, this script could be used to re-run the last 50 steps:

```
units           lj
atom_style      bond
pair_style      lj/cut 1.12
pair_modify     shift yes
bond_style      fene
special_bonds   0.0 1.0 1.0

read_data       tmp.restart.data

neighbor        0.4 bin
neigh_modify    every 1 delay 1

fix             1 all nve
fix             2 all langevin 1.0 1.0 10.0 904297

timestep        0.012

reset_timestep  50
run             50
```

Note that nearly all the settings specified in the original *in.chain* script must be repeated, except the *pair_coeff* and *bond_coeff* commands since the new data file lists the force field coefficients. Also, the *reset_timestep* command is used to tell LAMMPS the current timestep. This value is stored in restart files, but not in data files.

8.2.2 Visualize LAMMPS snapshots

LAMMPS itself does not do visualization, but snapshots from LAMMPS simulations can be visualized (and analyzed) in a variety of ways.

Mention dump image and dump movie.

LAMMPS snapshots are created by the *dump* command which can create files in several formats. The native LAMMPS dump format is a text file (see "dump atom" or "dump custom") which can be visualized by several popular visualization tools. The *dump image* and *dump movie* styles can output internally rendered images and convert a sequence of them to a movie during the MD run. Several programs included with LAMMPS as auxiliary tools can convert between LAMMPS format files and other formats. See the *Tools* doc page for details.

A Python-based toolkit distributed by our group can read native LAMMPS dump files, including custom dump files with additional columns of user-specified atom information, and convert them to various formats or pipe them into visualization software directly. See the Pizza.py WWW site for details. Specifically, Pizza.py can convert LAMMPS dump files into PDB, XYZ, Ensight, and VTK formats. Pizza.py can pipe LAMMPS dump files directly into the Raster3d and RasMol visualization programs. Pizza.py has tools that do interactive 3d OpenGL visualization and one that creates SVG images of dump file snapshots.

8.2.3 Run multiple simulations from one input script

This can be done in several ways. See the documentation for individual commands for more details on how these examples work.

If "multiple simulations" means continue a previous simulation for more timesteps, then you simply use the *run* command multiple times. For example, this script

```
units lj
atom_style atomic
read_data data.lj
```

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```
run 10000
run 10000
run 10000
run 10000
run 10000
```

would run 5 successive simulations of the same system for a total of 50,000 timesteps.

If you wish to run totally different simulations, one after the other, the *clear* command can be used in between them to re-initialize LAMMPS. For example, this script

```
units lj
atom_style atomic
read_data data.lj
run 10000
clear
units lj
atom_style atomic
read_data data.lj.new
run 10000
```

would run 2 independent simulations, one after the other.

For large numbers of independent simulations, you can use *variables* and the *next* and *jump* commands to loop over the same input script multiple times with different settings. For example, this script, named in.polymer

```
variable d index run1 run2 run3 run4 run5 run6 run7 run8
shell cd $d
read_data data.polymer
run 10000
shell cd ..
clear
next d
jump in.polymer
```

would run 8 simulations in different directories, using a data.polymer file in each directory. The same concept could be used to run the same system at 8 different temperatures, using a temperature variable and storing the output in different log and dump files, for example

```
variable a loop 8
variable t index 0.8 0.85 0.9 0.95 1.0 1.05 1.1 1.15
log log.$a
read data.polymer
velocity all create $t 352839
fix 1 all nvt $t $t 100.0
dump 1 all atom 1000 dump.$a
run 100000
clear
next t
next a
jump in.polymer
```

All of the above examples work whether you are running on 1 or multiple processors, but assumed you are running LAMMPS on a single partition of processors. LAMMPS can be run on multiple partitions via the *-partition command-line switch*.

In the last 2 examples, if LAMMPS were run on 3 partitions, the same scripts could be used if the "index" and "loop" variables were replaced with *universe*-style variables, as described in the *variable* command. Also, the "next

t" and "next a" commands would need to be replaced with a single "next a t" command. With these modifications, the 8 simulations of each script would run on the 3 partitions one after the other until all were finished. Initially, 3 simulations would be started simultaneously, one on each partition. When one finished, that partition would then start the 4th simulation, and so forth, until all 8 were completed.

8.2.4 Multi-replica simulations

Several commands in LAMMPS run multi-replica simulations, meaning that multiple instances (replicas) of your simulation are run simultaneously, with small amounts of data exchanged between replicas periodically.

These are the relevant commands:

- *neb* for nudged elastic band calculations
- *neb_spin* for magnetic nudged elastic band calculations
- *prd* for parallel replica dynamics
- *tad* for temperature accelerated dynamics
- *temper* for parallel tempering
- *fix pimd* for path-integral molecular dynamics (PIMD)

NEB is a method for finding transition states and barrier energies. PRD and TAD are methods for performing accelerated dynamics to find and perform infrequent events. Parallel tempering or replica exchange runs different replicas at a series of temperature to facilitate rare-event sampling.

These commands can only be used if LAMMPS was built with the REPLICA package. See the *Build package* doc page for more info.

PIMD runs different replicas whose individual particles are coupled together by springs to model a system or ring-polymers.

This commands can only be used if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

In all these cases, you must run with one or more processors per replica. The processors assigned to each replica are determined at run-time by using the *-partition command-line switch* to launch LAMMPS on multiple partitions, which in this context are the same as replicas. E.g. these commands:

```
mpirun -np 16 lmp_linux -partition 8x2 -in in.temper
mpirun -np 8 lmp_linux -partition 8x1 -in in.neb
```

would each run 8 replicas, on either 16 or 8 processors. Note the use of the *-in command-line switch* to specify the input script which is required when running in multi-replica mode.

Also note that with MPI installed on a machine (e.g. your desktop), you can run on more (virtual) processors than you have physical processors. Thus the above commands could be run on a single-processor (or few-processor) desktop so that you can run a multi-replica simulation on more replicas than you have physical processors.

8.2.5 Library interface to LAMMPS

As described on the *Build basics* doc page, LAMMPS can be built as a library, so that it can be called by another code, used in a *coupled manner* with other codes, or driven through a *Python interface*.

All of these methodologies use a C-style interface to LAMMPS that is provided in the files src/library.cpp and src/library.h. The functions therein have a C-style argument list, but contain C++ code you could write yourself in a C++ application that was invoking LAMMPS directly. The C++ code in the functions illustrates how to invoke internal LAMMPS operations. Note that LAMMPS classes are defined within a LAMMPS namespace (LAMMPS_NS) if you use them from another C++ application.

The examples/COUPLE and python/examples directories have example C++ and C and Python codes which show how a driver code can link to LAMMPS as a library, run LAMMPS on a subset of processors, grab data from LAMMPS, change it, and put it back into LAMMPS.

Thread-safety

LAMMPS has not initially been conceived as a thread-safe program, but over the years changes have been applied to replace operations that collide with creating multiple LAMMPS instances from multiple-threads of the same process with thread-safe alternatives. This primarily applies to the core LAMMPS code and less so on add-on packages, especially when those packages require additional code in the *lib* folder, interface LAMMPS to Fortran libraries, or the code uses static variables (like the USER-COLVARS package.

Another major issue to deal with is to correctly handle MPI. Creating a LAMMPS instance requires passing an MPI communicator, or it assumes the MPI_COMM_WORLD communicator, which spans all MPI processor ranks. When creating multiple LAMMPS object instances from different threads, this communicator has to be different for each thread or else collisions can happen, or it has to be guaranteed, that only one thread at a time is active. MPI communicators, however, are not a problem, if LAMMPS is compiled with the MPI STUBS library, which implies that there is no MPI communication and only 1 MPI rank.

Provided APIs

The file src/library.cpp contains the following functions for creating and destroying an instance of LAMMPS and sending it commands to execute. See the documentation in the src/library.cpp file for details.

Note: You can write code for additional functions as needed to define how your code talks to LAMMPS and add them to src/library.cpp and src/library.h, as well as to the *Python interface*. The added functions can access or change any internal LAMMPS data you wish.

```
void lammps_open(int, char **, MPI_Comm, void **)
void lammps_open_no_mpi(int, char **, void **)
void lammps_close(void *)
int lammps_version(void *)
void lammps_file(void *, char *)
char *lammps_command(void *, char *)
void lammps_commands_list(void *, int, char **)
void lammps_commands_string(void *, char *)
void lammps_free(void *)
```

The lammps_open() function is used to initialize LAMMPS, passing in a list of strings as if they were *command-line arguments* when LAMMPS is run in stand-alone mode from the command line, and a MPI communicator for LAMMPS to run under. It returns a ptr to the LAMMPS object that is created, and which is used in subsequent library calls. The lammps_open() function can be called multiple times, to create multiple instances of LAMMPS.

LAMMPS will run on the set of processors in the communicator. This means the calling code can run LAMMPS on all or a subset of processors. For example, a wrapper script might decide to alternate between LAMMPS and another code, allowing them both to run on all the processors. Or it might allocate half the processors to LAMMPS and half to the other code and run both codes simultaneously before syncing them up periodically. Or it might instantiate multiple instances of LAMMPS to perform different calculations.

The lammps_open_no_mpi() function is similar except that no MPI communicator is passed from the caller. Instead, MPI_COMM_WORLD is used to instantiate LAMMPS, and MPI is initialized if necessary.

The lammps_close() function is used to shut down an instance of LAMMPS and free all its memory.

The lammps_version() function can be used to determined the specific version of the underlying LAMMPS code. This is particularly useful when loading LAMMPS as a shared library via dlopen(). The code using the library interface can than use this information to adapt to changes to the LAMMPS command syntax between versions. The returned LAMMPS version code is an integer (e.g. 2 Sep 2015 results in 20150902) that grows with every new LAMMPS version.

The lammps_file(), lammps_command(), lammps_commands_list(), and lammps_commands_string() functions are used to pass one or more commands to LAMMPS to execute, the same as if they were coming from an input script.

Via these functions, the calling code can read or generate a series of LAMMPS commands one or multiple at a time and pass it through the library interface to setup a problem and then run it in stages. The caller can interleave the command function calls with operations it performs, calls to extract information from or set information within LAMMPS, or calls to another code's library.

The lammps_file() function passes the filename of an input script. The lammps_command() function passes a single command as a string. The lammps_commands_list() function passes multiple commands in a char** list. In both lammps_command() and lammps_commands_list(), individual commands may or may not have a trailing newline. The lammps_commands_string() function passes multiple commands concatenated into one long string, separated by newline characters. In both lammps_commands_list() and lammps_commands_string(), a single command can be spread across multiple lines, if the last printable character of all but the last line is "&", the same as if the lines appeared in an input script.

The lammps_free() function is a clean-up function to free memory that the library allocated previously via other function calls. See comments in src/library.cpp file for which other functions need this clean-up.

The file src/library.cpp also contains these functions for extracting information from LAMMPS and setting value within LAMMPS. Again, see the documentation in the src/library.cpp file for details, including which quantities can be queried by name:

```
int lammps_extract_setting(void *, char *)
void *lammps_extract_global(void *, char *)
void lammps_extract_box(void *, double *, double *,
                        double *, double *, double *, int *, int *)
void *lammps_extract_atom(void *, char *)
void *lammps_extract_compute(void *, char *, int, int)
void *lammps_extract_fix(void *, char *, int, int, int, int)
void *lammps_extract_variable(void *, char *, char *)
```

The extract_setting() function returns info on the size of data types (e.g. 32-bit or 64-bit atom IDs) used by the LAMMPS executable (a compile-time choice).

The other extract functions return a pointer to various global or per-atom quantities stored in LAMMPS or to values calculated by a compute, fix, or variable. The pointer returned by the extract_global() function can be used as a permanent reference to a value which may change. For the extract_atom() method, see the extract() method in the src/atom.cpp file for a list of valid per-atom properties. New names could easily be added if the property you want is not listed. For the other extract functions, the underlying storage may be reallocated as LAMMPS runs, so you need to re-call the function to assure a current pointer or returned value(s).

```
double lammps_get_thermo(void *, char *)
int lammps_get_natoms(void *)

int lammps_set_variable(void *, char *, char *)
void lammps_reset_box(void *, double *, double *, double, double, double)
```

The lammps_get_thermo() function returns the current value of a thermo keyword as a double precision value.

The lammps_get_natoms() function returns the total number of atoms in the system and can be used by the caller to allocate memory for the lammps_gather_atoms() and lammps_scatter_atoms() functions.

The lammps_set_variable() function can set an existing string-style variable to a new string value, so that subsequent LAMMPS commands can access the variable.

The lammps_reset_box() function resets the size and shape of the simulation box, e.g. as part of restoring a previously extracted and saved state of a simulation.

```
void lammps_gather_atoms(void *, char *, int, int, void *)
void lammps_gather_atoms_concat(void *, char *, int, int, void *)
void lammps_gather_atoms_subset(void *, char *, int, int, int, int *, void *)
void lammps_scatter_atoms(void *, char *, int, int, void *)
void lammps_scatter_atoms_subset(void *, char *, int, int, int, int *, void *)
```

The gather functions collect peratom info of the requested type (atom coords, atom types, forces, etc) from all processors, and returns the same vector of values to each calling processor. The scatter functions do the inverse. They distribute a vector of peratom values, passed by all calling processors, to individual atoms, which may be owned by different processors.

Warning: These functions are not compatible with the -DLAMMPS_BIGBIG setting when compiling LAMMPS. Dummy functions that result in an error message and abort will be substituted instead of resulting in random crashes and memory corruption.

The lammps_gather_atoms() function does this for all N atoms in the system, ordered by atom ID, from 1 to N. The lammps_gather_atoms_concat() function does it for all N atoms, but simply concatenates the subset of atoms owned by each processor. The resulting vector is not ordered by atom ID. Atom IDs can be requested by the same function if the caller needs to know the ordering. The lammps_gather_subset() function allows the caller to request values for only a subset of atoms (identified by ID). For all 3 gather function, per-atom image flags can be retrieved in 2 ways. If the count is specified as 1, they are returned in a packed format with all three image flags stored in a single integer. If the count is specified as 3, the values are unpacked into xyz flags by the library before returning them.

The lammps_scatter_atoms() function takes a list of values for all N atoms in the system, ordered by atom ID, from 1 to N, and assigns those values to each atom in the system. The lammps_scatter_atoms_subset() function takes a subset of IDs as an argument and only scatters those values to the owning atoms.

```
void lammps_create_atoms(void *, int, tagint *, int *, double *, double *,
                         imageint *, int)
```

The lammps_create_atoms() function takes a list of N atoms as input with atom types and coords (required), an optionally atom IDs and velocities and image flags. It uses the coords of each atom to assign it as a new atom to the processor that owns it. This function is useful to add atoms to a simulation or (in tandem with lammps_reset_box()) to restore a previously extracted and saved state of a simulation. Additional properties for the new atoms can then be assigned via the lammps_scatter_atoms() or lammps_extract_atom() functions.

8.2.6 Coupling LAMMPS to other codes

LAMMPS is designed to allow it to be coupled to other codes. For example, a quantum mechanics code might compute forces on a subset of atoms and pass those forces to LAMMPS. Or a continuum finite element (FE) simulation might use atom positions as boundary conditions on FE nodal points, compute a FE solution, and return interpolated forces on MD atoms.

LAMMPS can be coupled to other codes in at least 4 ways. Each has advantages and disadvantages, which you will have to think about in the context of your application.

---

(1) Define a new *fix* command that calls the other code. In this scenario, LAMMPS is the driver code. During its timestepping, the fix is invoked, and can make library calls to the other code, which has been linked to LAMMPS as a library. This is the way the POEMS package that performs constrained rigid-body motion on groups of atoms is hooked to LAMMPS. See the *fix poems* command for more details. See the *Modify* doc pages for info on how to add a new fix to LAMMPS.

---

(2) Define a new LAMMPS command that calls the other code. This is conceptually similar to method (1), but in this case LAMMPS and the other code are on a more equal footing. Note that now the other code is not called during the timestepping of a LAMMPS run, but between runs. The LAMMPS input script can be used to alternate LAMMPS runs with calls to the other code, invoked via the new command. The *run* command facilitates this with its *every* option, which makes it easy to run a few steps, invoke the command, run a few steps, invoke the command, etc.

In this scenario, the other code can be called as a library, as in (1), or it could be a stand-alone code, invoked by a system() call made by the command (assuming your parallel machine allows one or more processors to start up another program). In the latter case the stand-alone code could communicate with LAMMPS through files that the command writes and reads.

See the *Modify command* doc page for info on how to add a new command to LAMMPS.

---

(3) Use LAMMPS as a library called by another code. In this case the other code is the driver and calls LAMMPS as needed. Or a wrapper code could link and call both LAMMPS and another code as libraries. Again, the *run* command has options that allow it to be invoked with minimal overhead (no setup or clean-up) if you wish to do multiple short runs, driven by another program.

Examples of driver codes that call LAMMPS as a library are included in the examples/COUPLE directory of the LAMMPS distribution; see examples/COUPLE/README for more details:

- simple: simple driver programs in C++ and C which invoke LAMMPS as a library
- plugin: simple driver program in C which invokes LAMMPS as a plugin from a shared library.
- lammps_quest: coupling of LAMMPS and Quest, to run classical MD with quantum forces calculated by a density functional code
- lammps_spparks: coupling of LAMMPS and SPPARKS, to couple a kinetic Monte Carlo model for grain growth using MD to calculate strain induced across grain boundaries

The *Build basics* doc page describes how to build LAMMPS as a library. Once this is done, you can interface with LAMMPS either via C++, C, Fortran, or Python (or any other language that supports a vanilla C-like interface). For example, from C++ you could create one (or more) "instances" of LAMMPS, pass it an input script to process, or execute individual commands, all by invoking the correct class methods in LAMMPS. From C or Fortran you can make function calls to do the same things. See the *Python* doc pages for a description of the Python wrapper provided with LAMMPS that operates through the LAMMPS library interface.

The files src/library.cpp and library.h contain the C-style interface to LAMMPS. See the *Howto library* doc page for a description of the interface and how to extend it for your needs.

Note that the lammps_open() function that creates an instance of LAMMPS takes an MPI communicator as an argument. This means that instance of LAMMPS will run on the set of processors in the communicator. Thus the calling code can run LAMMPS on all or a subset of processors. For example, a wrapper script might decide to alternate between LAMMPS and another code, allowing them both to run on all the processors. Or it might allocate half the processors to LAMMPS and half to the other code and run both codes simultaneously before syncing them up periodically. Or it might instantiate multiple instances of LAMMPS to perform different calculations.

---

(4) Couple LAMMPS with another code in a client/server mode. This is described on the *Howto client/server* doc page.

8.2.7 Using LAMMPS in client/server mode

Client/server coupling of two codes is where one code is the "client" and sends request messages to a "server" code. The server responds to each request with a reply message. This enables the two codes to work in tandem to perform a simulation. LAMMPS can act as either a client or server code.

Some advantages of client/server coupling are that the two codes run as stand-alone executables; they are not linked together. Thus neither code needs to have a library interface. This often makes it easier to run the two codes on different numbers of processors. If a message protocol (format and content) is defined for a particular kind of simulation, then in principle any code that implements the client-side protocol can be used in tandem with any code that implements the server-side protocol, without the two codes needing to know anything more specific about each other.

A simple example of client/server coupling is where LAMMPS is the client code performing MD timestepping. Each timestep it sends a message to a server quantum code containing current coords of all the atoms. The quantum code computes energy and forces based on the coords. It returns them as a message to LAMMPS, which completes the timestep.

A more complex example is where LAMMPS is the client code and processes a series of data files, sending each configuration to a quantum code to compute energy and forces. Or LAMMPS runs dynamics with an atomistic force field, but pauses every N steps to ask the quantum code to compute energy and forces.

Alternate methods for code coupling with LAMMPS are described on the *Howto couple* doc page.

The protocol for using LAMMPS as a client is to use these 3 commands in this order (other commands may come in between):

- *message client* # initiate client/server interaction
- *fix client/md* # any client fix which makes specific requests to the server
- *message quit* # terminate client/server interaction

In between the two message commands, a client fix command and *unfix* command can be used multiple times. Similarly, this sequence of 3 commands can be repeated multiple times, assuming the server program operates in a similar fashion, to initiate and terminate client/server communication.

The protocol for using LAMMPS as a server is to use these 2 commands in this order (other commands may come in between):

- *message server* # initiate client/server interaction
- *server md* # any server command which responds to specific requests from the client

This sequence of 2 commands can be repeated multiple times, assuming the client program operates in a similar fashion, to initiate and terminate client/server communication.

LAMMPS support for client/server coupling is in its *MESSAGE package* which implements several commands that enable LAMMPS to act as a client or server, as discussed below. The MESSAGE package also wraps a client/server library called CSlib which enables two codes to exchange messages in different ways, either via files, sockets, or MPI.

The CSlib is provided with LAMMPS in the lib/message dir. The CSlib has its own website with documentation and test programs.

Note: For client/server coupling to work between LAMMPS and another code, the other code also has to use the CSlib. This can sometimes be done without any modifications to the other code by simply wrapping it with a Python script that exchanges CSlib messages with LAMMPS and prepares input for or processes output from the other code. The other code also has to implement a matching protocol for the format and content of messages that LAMMPS exchanges with it.

These are the commands currently in the MESSAGE package for two protocols, MD and MC (Monte Carlo). New protocols can easily be defined and added to this directory, where LAMMPS acts as either the client or server.

- *message*
- *fix client md* = LAMMPS is a client for running MD
- *server md* = LAMMPS is a server for computing MD forces
- *server mc* = LAMMPS is a server for computing a Monte Carlo energy

The server doc files give details of the message protocols for data that is exchanged between the client and server.

These example directories illustrate how to use LAMMPS as either a client or server code:

- examples/message
- examples/COUPLE/README
- examples/COUPLE/lammps_mc
- examples/COUPLE/lammps_nwchem
- examples/COUPLE/lammps_vasp

The examples/message directory couples a client instance of LAMMPS to a server instance of LAMMPS.

The files in the *lammps_mc* folder show how to couple LAMMPS as a server to a simple Monte Carlo client code as the driver.

The files in the *lammps_nwchem* folder show how to couple LAMMPS as a client code running MD timestepping to NWChem acting as a server providing quantum DFT forces, through a Python wrapper script on NWChem.

The files in the *lammps_vasp* folder show how to couple LAMMPS as a client code running MD timestepping to VASP acting as a server providing quantum DFT forces, through a Python wrapper script on VASP.

Here is how to launch a client and server code together for any of the 4 modes of message exchange that the *message* command and the CSlib support. Here LAMMPS is used as both the client and server code. Another code could be substituted for either.

The examples below show launching both codes from the same window (or batch script), using the "&" character to launch the first code in the background. For all modes except *mpi/one*, you could also launch the codes in separate windows on your desktop machine. It does not matter whether you launch the client or server first.

In these examples either code can be run on one or more processors. If running in a non-MPI mode (file or zmq) you can launch a code on a single processor without using mpirun.

IMPORTANT: If you run in mpi/two mode, you must launch both codes via mpirun, even if one or both of them runs on a single processor. This is so that MPI can figure out how to connect both MPI processes together to exchange MPI messages between them.

For message exchange in *file*, *zmq*, or *mpi/two* modes:

```
% mpirun -np 1 lmp_mpi -log log.client < in.client &
% mpirun -np 2 lmp_mpi -log log.server < in.server

% mpirun -np 4 lmp_mpi -log log.client < in.client &
% mpirun -np 1 lmp_mpi -log log.server < in.server

% mpirun -np 2 lmp_mpi -log log.client < in.client &
% mpirun -np 4 lmp_mpi -log log.server < in.server
```

For message exchange in *mpi/one* mode:

Launch both codes in a single mpirun command:

```
mpirun -np 2 lmp_mpi -mpicolor 0 -in in.message.client -log log.client : -np 4 lmp_
↪mpi -mpicolor 1 -in in.message.server -log log.server
```

The two -np values determine how many procs the client and the server run on.

A LAMMPS executable run in this manner must use the -mpicolor color command-line option as their its option, where color is an integer label that will be used to distinguish one executable from another in the multiple executables that the mpirun command launches. In this example the client was colored with a 0, and the server with a 1.

8.3 Settings howto

8.3.1 2d simulations

Use the *dimension* command to specify a 2d simulation.

Make the simulation box periodic in z via the *boundary* command. This is the default.

If using the *create box* command to define a simulation box, set the z dimensions narrow, but finite, so that the create_atoms command will tile the 3d simulation box with a single z plane of atoms - e.g.

```
:doc:`create box <create_box>` 1 -10 10 -10 10 -0.25 0.25
```

If using the *read data* command to read in a file of atom coordinates, set the "zlo zhi" values to be finite but narrow, similar to the create_box command settings just described. For each atom in the file, assign a z coordinate so it falls inside the z-boundaries of the box - e.g. 0.0.

Use the *fix enforce2d* command as the last defined fix to insure that the z-components of velocities and forces are zeroed out every timestep. The reason to make it the last fix is so that any forces induced by other fixes will be zeroed out.

Many of the example input scripts included in the LAMMPS distribution are for 2d models.

Note: Some models in LAMMPS treat particles as finite-size spheres, as opposed to point particles. See the *atom_style sphere* and *fix nve/sphere* commands for details. By default, for 2d simulations, such particles will still be modeled as 3d spheres, not 2d discs (circles), meaning their moment of inertia will be that of a sphere. If you wish to model them as 2d discs, see the *set density/disc* command and the *disc* option for the *fix nve/sphere*, *fix nvt/sphere*, *fix nph/sphere*, *fix npt/sphere* commands.

8.3.2 Triclinic (non-orthogonal) simulation boxes

By default, LAMMPS uses an orthogonal simulation box to encompass the particles. The *boundary* command sets the boundary conditions of the box (periodic, non-periodic, etc). The orthogonal box has its "origin" at (xlo,ylo,zlo) and is defined by 3 edge vectors starting from the origin given by **a** = (xhi-xlo,0,0); **b** = (0,yhi-ylo,0); **c** = (0,0,zhi-zlo). The 6 parameters (xlo,xhi,ylo,yhi,zlo,zhi) are defined at the time the simulation box is created, e.g. by the *create_box* or *read_data* or *read_restart* commands. Additionally, LAMMPS defines box size parameters lx,ly,lz where lx = xhi-xlo, and similarly in the y and z dimensions. The 6 parameters, as well as lx,ly,lz, can be output via the *thermo_style custom* command.

LAMMPS also allows simulations to be performed in triclinic (non-orthogonal) simulation boxes shaped as a parallelepiped with triclinic symmetry. The parallelepiped has its "origin" at (xlo,ylo,zlo) and is defined by 3 edge vectors starting from the origin given by **a** = (xhi-xlo,0,0); **b** = (xy,yhi-ylo,0); **c** = (xz,yz,zhi-zlo). *xy,xz,yz* can be 0.0 or positive or negative values and are called "tilt factors" because they are the amount of displacement applied to faces of an originally orthogonal box to transform it into the parallelepiped. In LAMMPS the triclinic simulation box edge vectors **a**, **b**, and **c** cannot be arbitrary vectors. As indicated, **a** must lie on the positive x axis. **b** must lie in the xy plane, with strictly positive y component. **c** may have any orientation with strictly positive z component. The requirement that **a**, **b**, and **c** have strictly positive x, y, and z components, respectively, ensures that **a**, **b**, and **c** form a complete right-handed basis. These restrictions impose no loss of generality, since it is possible to rotate/invert any set of 3 crystal basis vectors so that they conform to the restrictions.

For example, assume that the 3 vectors **A**,**B**,**C** are the edge vectors of a general parallelepiped, where there is no restriction on **A**,**B**,**C** other than they form a complete right-handed basis i.e. **A** x **B** . **C** > 0. The equivalent LAMMPS **a**,**b**,**c** are a linear rotation of **A**, **B**, and **C** and can be computed as follows:

$$
\begin{aligned}
\begin{pmatrix}\mathbf{a} & \mathbf{b} & \mathbf{c}\end{pmatrix} = \begin{pmatrix} a_x & b_x & c_x \\ 0 & b_y & c_y \\ 0 & 0 & c_z \end{pmatrix} \\
a_x =& A \\
b_x =& \mathbf{B}\cdot\hat{\mathbf{A}} \quad = \quad B\cos\gamma \\
b_y =& |\hat{\mathbf{A}}\times\mathbf{B}| \quad = \quad B\sin\gamma \quad = \quad \sqrt{B^2 - {b_x}^2} \\
c_x =& \mathbf{C}\cdot\hat{\mathbf{A}} \quad = \quad C\cos\beta \\
c_y =& \mathbf{C}\cdot(\widehat{\mathbf{A}\times\mathbf{B}})\times\hat{\mathbf{A}} \quad = \quad \frac{\mathbf{B}\cdot\mathbf{C} - b_x c_x}{b_y} \\
c_z =& |\mathbf{C}\cdot(\widehat{\mathbf{A}\times\mathbf{B}})| \quad = \quad \sqrt{C^2 - {c_x}^2 - {c_y}^2}
\end{aligned}
$$

where A = | **A** | indicates the scalar length of **A**. The hat symbol (^) indicates the corresponding unit vector. β and γ are angles between the vectors described below. Note that by construction, **a**, **b**, and **c** have strictly positive x, y, and z components, respectively. If it should happen that **A**, **B**, and **C** form a left-handed basis, then the above equations are not valid for **c**. In this case, it is necessary to first apply an inversion. This can be achieved by interchanging two basis vectors or by changing the sign of one of them.

For consistency, the same rotation/inversion applied to the basis vectors must also be applied to atom positions, velocities, and any other vector quantities. This can be conveniently achieved by first converting to fractional coordinates in the old basis and then converting to distance coordinates in the new basis. The transformation is given by the following equation:

$$
\mathbf{x} = \begin{pmatrix}\mathbf{a} & \mathbf{b} & \mathbf{c}\end{pmatrix} \cdot \frac{1}{V} \begin{pmatrix} \mathbf{B}\times\mathbf{C} \\ \mathbf{C}\times\mathbf{A} \\ \mathbf{A}\times\mathbf{B} \end{pmatrix} \cdot \mathbf{X}
$$

where V is the volume of the box, **X** is the original vector quantity and **x** is the vector in the LAMMPS basis.

There is no requirement that a triclinic box be periodic in any dimension, though it typically should be in at least the 2nd dimension of the tilt (y in xy) if you want to enforce a shift in periodic boundary conditions across that boundary.

Some commands that work with triclinic boxes, e.g. the *fix deform* and *fix npt* commands, require periodicity or non-shrink-wrap boundary conditions in specific dimensions. See the command doc pages for details.

The 9 parameters (xlo,xhi,ylo,yhi,zlo,zhi,xy,xz,yz) are defined at the time the simulation box is created. This happens in one of 3 ways. If the *create_box* command is used with a region of style *prism*, then a triclinic box is setup. See the *region* command for details. If the *read_data* command is used to define the simulation box, and the header of the data file contains a line with the "xy xz yz" keyword, then a triclinic box is setup. See the *read_data* command for details. Finally, if the *read_restart* command reads a restart file which was written from a simulation using a triclinic box, then a triclinic box will be setup for the restarted simulation.

Note that you can define a triclinic box with all 3 tilt factors = 0.0, so that it is initially orthogonal. This is necessary if the box will become non-orthogonal, e.g. due to the *fix npt* or *fix deform* commands. Alternatively, you can use the *change_box* command to convert a simulation box from orthogonal to triclinic and vice versa.

As with orthogonal boxes, LAMMPS defines triclinic box size parameters lx,ly,lz where lx = xhi-xlo, and similarly in the y and z dimensions. The 9 parameters, as well as lx,ly,lz, can be output via the *thermo_style custom* command.

To avoid extremely tilted boxes (which would be computationally inefficient), LAMMPS normally requires that no tilt factor can skew the box more than half the distance of the parallel box length, which is the 1st dimension in the tilt factor (x for xz). This is required both when the simulation box is created, e.g. via the *create_box* or *read_data* commands, as well as when the box shape changes dynamically during a simulation, e.g. via the *fix deform* or *fix npt* commands.

For example, if xlo = 2 and xhi = 12, then the x box length is 10 and the xy tilt factor must be between -5 and 5. Similarly, both xz and yz must be between -(xhi-xlo)/2 and +(yhi-ylo)/2. Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = . . . , -15, -5, 5, 15, 25, . . . are geometrically all equivalent. If the box tilt exceeds this limit during a dynamics run (e.g. via the *fix deform* command), then the box is "flipped" to an equivalent shape with a tilt factor within the bounds, so the run can continue. See the *fix deform* doc page for further details.

One exception to this rule is if the 1st dimension in the tilt factor (x for xy) is non-periodic. In that case, the limits on the tilt factor are not enforced, since flipping the box in that dimension does not change the atom positions due to non-periodicity. In this mode, if you tilt the system to extreme angles, the simulation will simply become inefficient, due to the highly skewed simulation box.

The limitation on not creating a simulation box with a tilt factor skewing the box more than half the distance of the parallel box length can be overridden via the *box* command. Setting the *tilt* keyword to *large* allows any tilt factors to be specified.

Box flips that may occur using the *fix deform* or *fix npt* commands can be turned off using the *flip no* option with either of the commands.

Note that if a simulation box has a large tilt factor, LAMMPS will run less efficiently, due to the large volume of communication needed to acquire ghost atoms around a processor's irregular-shaped sub-domain. For extreme values of tilt, LAMMPS may also lose atoms and generate an error.

Triclinic crystal structures are often defined using three lattice constants a, b, and c, and three angles α, β, and γ. Note that in this nomenclature, the a, b, and c lattice constants are the scalar lengths of the edge vectors **a**, **b**, and **c** defined above. The relationship between these 6 quantities (a, b, c, α, β, γ) and the LAMMPS box sizes (lx,ly,lz) =

(xhi-xlo,yhi-ylo,zhi-zlo) and tilt factors (xy,xz,yz) is as follows:

$$
\begin{aligned}
a =& \mathrm{lx} \\
b^2 =& \mathrm{ly}^2 + \mathrm{xy}^2 \\
c^2 =& \mathrm{lz}^2 + \mathrm{xz}^2 + \mathrm{yz}^2 \\
\cos\alpha =& \frac{\mathrm{xy} * \mathrm{xz} + \mathrm{ly} * \mathrm{yz}}{b * c} \\
\cos\beta =& \frac{\mathrm{xz}}{c} \\
\cos\gamma =& \frac{\mathrm{xy}}{b}
\end{aligned}
$$

The inverse relationship can be written as follows:

$$
\begin{aligned}
\mathrm{lx} =& a \\
\mathrm{xy} =& b\cos\gamma \\
\mathrm{xz} =& c\cos\beta \\
\mathrm{ly}^2 =& b^2 - \mathrm{xy}^2 \\
\mathrm{yz} =& \frac{b * c\cos\alpha - \mathrm{xy} * \mathrm{xz}}{\mathrm{ly}} \\
\mathrm{lz}^2 =& c^2 - \mathrm{xz}^2 - \mathrm{yz}^2
\end{aligned}
$$

The values of a, b, c , α , β, and γ can be printed out or accessed by computes using the *thermo_style custom* keywords *cella*, *cellb*, *cellc*, *cellalpha*, *cellbeta*, *cellgamma*, respectively.

As discussed on the *dump* command doc page, when the BOX BOUNDS for a snapshot is written to a dump file for a triclinic box, an orthogonal bounding box which encloses the triclinic simulation box is output, along with the 3 tilt factors (xy, xz, yz) of the triclinic box, formatted as follows:

```
ITEM: BOX BOUNDS xy xz yz
xlo_bound xhi_bound xy
ylo_bound yhi_bound xz
zlo_bound zhi_bound yz
```

This bounding box is convenient for many visualization programs and is calculated from the 9 triclinic box parameters (xlo,xhi,ylo,yhi,zlo,zhi,xy,xz,yz) as follows:

```
xlo_bound = xlo + MIN(0.0,xy,xz,xy+xz)
xhi_bound = xhi + MAX(0.0,xy,xz,xy+xz)
ylo_bound = ylo + MIN(0.0,yz)
yhi_bound = yhi + MAX(0.0,yz)
zlo_bound = zlo
zhi_bound = zhi
```

These formulas can be inverted if you need to convert the bounding box back into the triclinic box parameters, e.g. xlo = xlo_bound - MIN(0.0,xy,xz,xy+xz).

One use of triclinic simulation boxes is to model solid-state crystals with triclinic symmetry. The *lattice* command can be used with non-orthogonal basis vectors to define a lattice that will tile a triclinic simulation box via the *create_atoms* command.

A second use is to run Parrinello-Rahman dynamics via the *fix npt* command, which will adjust the xy, xz, yz tilt factors to compensate for off-diagonal components of the pressure tensor. The analog for an *energy minimization* is the *fix box/relax* command.

A third use is to shear a bulk solid to study the response of the material. The *fix deform* command can be used for this purpose. It allows dynamic control of the xy, xz, yz tilt factors as a simulation runs. This is discussed in the next section on non-equilibrium MD (NEMD) simulations.

8.3.3 Thermostats

Thermostatting means controlling the temperature of particles in an MD simulation. *Barostatting* means controlling the pressure. Since the pressure includes a kinetic component due to particle velocities, both these operations require calculation of the temperature. Typically a target temperature (T) and/or pressure (P) is specified by the user, and the thermostat or barostat attempts to equilibrate the system to the requested T and/or P.

Thermostatting in LAMMPS is performed by *fixes*, or in one case by a pair style. Several thermostatting fixes are available: Nose-Hoover (nvt), Berendsen, CSVR, Langevin, and direct rescaling (temp/rescale). Dissipative particle dynamics (DPD) thermostatting can be invoked via the *dpd/tstat* pair style:

- *fix nvt*
- *fix nvt/sphere*
- *fix nvt/asphere*
- *fix nvt/sllod*
- *fix temp/berendsen*
- *fix temp/csvr*
- *fix langevin*
- *fix temp/rescale*
- *pair_style dpd/tstat*

Fix nvt only thermostats the translational velocity of particles. *Fix nvt/sllod* also does this, except that it subtracts out a velocity bias due to a deforming box and integrates the SLLOD equations of motion. See the *Howto nemd* doc page for further details. *Fix nvt/sphere* and *fix nvt/asphere* thermostat not only translation velocities but also rotational velocities for spherical and aspherical particles.

Note: A recent (2017) book by *(Daivis and Todd)* discusses use of the SLLOD method and non-equilibrium MD (NEMD) thermostatting generally, for both simple and complex fluids, e.g. molecular systems. The latter can be tricky to do correctly.

DPD thermostatting alters pairwise interactions in a manner analogous to the per-particle thermostatting of *fix langevin*.

Any of the thermostatting fixes can use *temperature computes* that remove bias which has two effects. First, the current calculated temperature, which is compared to the requested target temperature, is calculated with the velocity bias removed. Second, the thermostat adjusts only the thermal temperature component of the particle's velocities, which are the velocities with the bias removed. The removed bias is then added back to the adjusted velocities. See the doc pages for the individual fixes and for the *fix_modify* command for instructions on how to assign a temperature compute to a thermostatting fix. For example, you can apply a thermostat to only the x and z components of velocity by using it in conjunction with *compute temp/partial*. Of you could thermostat only the thermal temperature of a streaming flow of particles without affecting the streaming velocity, by using *compute temp/profile*.

Note: Only the nvt fixes perform time integration, meaning they update the velocities and positions of particles due to forces and velocities respectively. The other thermostat fixes only adjust velocities; they do NOT perform time integration updates. Thus they should be used in conjunction with a constant NVE integration fix such as these:

- *fix nve*
- *fix nve/sphere*
- *fix nve/asphere*

Thermodynamic output, which can be setup via the *thermo_style* command, often includes temperature values. As explained on the doc page for the *thermo_style* command, the default temperature is setup by the thermo command itself. It is NOT the temperature associated with any thermostatting fix you have defined or with any compute you have defined that calculates a temperature. The doc pages for the thermostatting fixes explain the ID of the temperature compute they create. Thus if you want to view these temperatures, you need to specify them explicitly via the *thermo_style custom* command. Or you can use the *thermo_modify* command to re-define what temperature compute is used for default thermodynamic output.

(Daivis and Todd) Daivis and Todd, Nonequilibrium Molecular Dynamics (book), Cambridge University Press, https://doi.org/10.1017/9781139017848, (2017).

8.3.4 Barostats

Barostatting means controlling the pressure in an MD simulation. *Thermostatting* means controlling the temperature of the particles. Since the pressure includes a kinetic component due to particle velocities, both these operations require calculation of the temperature. Typically a target temperature (T) and/or pressure (P) is specified by the user, and the thermostat or barostat attempts to equilibrate the system to the requested T and/or P.

Barostatting in LAMMPS is performed by *fixes*. Two barostatting methods are currently available: Nose-Hoover (npt and nph) and Berendsen:

- *fix npt*
- *fix npt/sphere*
- *fix npt/asphere*
- *fix nph*
- *fix press/berendsen*

The *fix npt* commands include a Nose-Hoover thermostat and barostat. *Fix nph* is just a Nose/Hoover barostat; it does no thermostatting. Both *fix nph* and *fix press/berendsen* can be used in conjunction with any of the thermostatting fixes.

As with the *thermostats*, *fix npt* and *fix nph* only use translational motion of the particles in computing T and P and performing thermo/barostatting. *Fix npt/sphere* and *fix npt/asphere* thermo/barostat using not only translation velocities but also rotational velocities for spherical and aspherical particles.

All of the barostatting fixes use the *compute pressure* compute to calculate a current pressure. By default, this compute is created with a simple *compute temp* (see the last argument of the *compute pressure* command), which is used to calculated the kinetic component of the pressure. The barostatting fixes can also use temperature computes that remove bias for the purpose of computing the kinetic component which contributes to the current pressure. See the doc pages for the individual fixes and for the *fix_modify* command for instructions on how to assign a temperature or pressure compute to a barostatting fix.

Note: As with the thermostats, the Nose/Hoover methods (*fix npt* and *fix nph*) perform time integration. *Fix press/berendsen* does NOT, so it should be used with one of the constant NVE fixes or with one of the NVT fixes.

Thermodynamic output, which can be setup via the *thermo_style* command, often includes pressure values. As explained on the doc page for the *thermo_style* command, the default pressure is setup by the thermo command itself. It is NOT the pressure associated with any barostatting fix you have defined or with any compute you have defined that calculates a pressure. The doc pages for the barostatting fixes explain the ID of the pressure compute they create. Thus if you want to view these pressures, you need to specify them explicitly via the *thermo_style custom* command. Or you can use the *thermo_modify* command to re-define what pressure compute is used for default thermodynamic output.

8.3.5 Walls

Walls in an MD simulation are typically used to bound particle motion, i.e. to serve as a boundary condition.

Walls in LAMMPS can be of rough (made of particles) or idealized surfaces. Ideal walls can be smooth, generating forces only in the normal direction, or frictional, generating forces also in the tangential direction.

Rough walls, built of particles, can be created in various ways. The particles themselves can be generated like any other particle, via the *lattice* and *create_atoms* commands, or read in via the *read_data* command.

Their motion can be constrained by many different commands, so that they do not move at all, move together as a group at constant velocity or in response to a net force acting on them, move in a prescribed fashion (e.g. rotate around a point), etc. Note that if a time integration fix like *fix nve* or *fix nvt* is not used with the group that contains wall particles, their positions and velocities will not be updated.

- *fix aveforce* - set force on particles to average value, so they move together
- *fix setforce* - set force on particles to a value, e.g. 0.0
- *fix freeze* - freeze particles for use as granular walls
- *fix nve/noforce* - advect particles by their velocity, but without force
- *fix move* - prescribe motion of particles by a linear velocity, oscillation, rotation, variable

The *fix move* command offers the most generality, since the motion of individual particles can be specified with *variable* formula which depends on time and/or the particle position.

For rough walls, it may be useful to turn off pairwise interactions between wall particles via the *neigh_modify exclude* command.

Rough walls can also be created by specifying frozen particles that do not move and do not interact with mobile particles, and then tethering other particles to the fixed particles, via a *bond*. The bonded particles do interact with other mobile particles.

Idealized walls can be specified via several fix commands. *Fix wall/gran* creates frictional walls for use with granular particles; all the other commands create smooth walls.

- *fix wall/reflect* - reflective flat walls
- *fix wall/lj93* - flat walls, with Lennard-Jones 9/3 potential
- *fix wall/lj126* - flat walls, with Lennard-Jones 12/6 potential
- *fix wall/colloid* - flat walls, with *pair_style colloid* potential
- *fix wall/harmonic* - flat walls, with repulsive harmonic spring potential
- *fix wall/morse* - flat walls, with Morse potential
- *fix wall/region* - use region surface as wall
- *fix wall/gran* - flat or curved walls with *pair_style granular* potential

The *lj93*, *lj126*, *colloid*, *harmonic*, and *morse* styles all allow the flat walls to move with a constant velocity, or oscillate in time. The *fix wall/region* command offers the most generality, since the region surface is treated as a wall, and the geometry of the region can be a simple primitive volume (e.g. a sphere, or cube, or plane), or a complex volume made from the union and intersection of primitive volumes. *Regions* can also specify a volume "interior" or "exterior" to the specified primitive shape or *union* or *intersection*. *Regions* can also be "dynamic" meaning they move with constant velocity, oscillate, or rotate.

The only frictional idealized walls currently in LAMMPS are flat or curved surfaces specified by the *fix wall/gran* command. At some point we plan to allow regoin surfaces to be used as frictional walls, as well as triangulated surfaces.

8.3.6 NEMD simulations

Non-equilibrium molecular dynamics or NEMD simulations are typically used to measure a fluid's rheological properties such as viscosity. In LAMMPS, such simulations can be performed by first setting up a non-orthogonal simulation box (see the preceding Howto section).

A shear strain can be applied to the simulation box at a desired strain rate by using the *fix deform* command. The *fix nvt/sllod* command can be used to thermostat the sheared fluid and integrate the SLLOD equations of motion for the system. Fix nvt/sllod uses *compute temp/deform* to compute a thermal temperature by subtracting out the streaming velocity of the shearing atoms. The velocity profile or other properties of the fluid can be monitored via the *fix ave/chunk* command.

Note: A recent (2017) book by *(Daivis and Todd)* discusses use of the SLLOD method and non-equilibrium MD (NEMD) thermostatting generally, for both simple and complex fluids, e.g. molecular systems. The latter can be tricky to do correctly.

As discussed in the previous section on non-orthogonal simulation boxes, the amount of tilt or skew that can be applied is limited by LAMMPS for computational efficiency to be 1/2 of the parallel box length. However, *fix deform* can continuously strain a box by an arbitrary amount. As discussed in the *fix deform* command, when the tilt value reaches a limit, the box is flipped to the opposite limit which is an equivalent tiling of periodic space. The strain rate can then continue to change as before. In a long NEMD simulation these box re-shaping events may occur many times.

In a NEMD simulation, the "remap" option of *fix deform* should be set to "remap v", since that is what *fix nvt/sllod* assumes to generate a velocity profile consistent with the applied shear strain rate.

An alternative method for calculating viscosities is provided via the *fix viscosity* command.

NEMD simulations can also be used to measure transport properties of a fluid through a pore or channel. Simulations of steady-state flow can be performed using the *fix flow/gauss* command.

(Daivis and Todd) Daivis and Todd, Nonequilibrium Molecular Dynamics (book), Cambridge University Press, https://doi.org/10.1017/9781139017848, (2017).

8.3.7 Long-range dispersion settings

The PPPM method computes interactions by splitting the pair potential into two parts, one of which is computed in a normal pairwise fashion, the so-called real-space part, and one of which is computed using the Fourier transform, the so called reciprocal-space or kspace part. For both parts, the potential is not computed exactly but is approximated. Thus, there is an error in both parts of the computation, the real-space and the kspace error. The just mentioned facts are true both for the PPPM for Coulomb as well as dispersion interactions. The deciding difference - and also the reason why the parameters for pppm/disp have to be selected with more care - is the impact of the errors on the results: The kspace error of the PPPM for Coulomb and dispersion interaction and the real-space error of the PPPM for Coulomb interaction have the character of noise. In contrast, the real-space error of the PPPM for dispersion has a clear physical interpretation: the underprediction of cohesion. As a consequence, the real-space error has a much stronger effect than the kspace error on simulation results for pppm/disp. Parameters must thus be chosen in a way that this error is much smaller than the kspace error.

When using pppm/disp and not making any specifications on the PPPM parameters via the kspace modify command, parameters will be tuned such that the real-space error and the kspace error are equal. This will result in simulations that are either inaccurate or slow, both of which is not desirable. For selecting parameters for the pppm/disp that provide fast and accurate simulations, there are two approaches, which both have their up- and downsides.

The first approach is to set desired real-space an kspace accuracies via the *kspace_modify force/disp/real* and *kspace_modify force/disp/kspace* commands. Note that the accuracies have to be specified in force units and are

thus dependent on the chosen unit settings. For real units, 0.0001 and 0.002 seem to provide reasonable accurate and efficient computations for the real-space and kspace accuracies. 0.002 and 0.05 work well for most systems using lj units. PPPM parameters will be generated based on the desired accuracies. The upside of this approach is that it usually provides a good set of parameters and will work for both the *kspace_modify diff ad* and *kspace_modify diff ik* options. The downside of the method is that setting the PPPM parameters will take some time during the initialization of the simulation.

The second approach is to set the parameters for the pppm/disp explicitly using the *kspace_modify mesh/disp*, *kspace_modify order/disp*, and *kspace_modify gewald/disp* commands. This approach requires a more experienced user who understands well the impact of the choice of parameters on the simulation accuracy and performance. This approach provides a fast initialization of the simulation. However, it is sensitive to errors: A combination of parameters that will perform well for one system might result in far-from-optimal conditions for other simulations. For example, parameters that provide accurate and fast computations for all-atomistic force fields can provide insufficient accuracy or united-atomistic force fields (which is related to that the latter typically have larger dispersion coefficients).

To avoid inaccurate or inefficient simulations, the pppm/disp stops simulations with an error message if no action is taken to control the PPPM parameters. If the automatic parameter generation is desired and real-space and kspace accuracies are desired to be equal, this error message can be suppressed using the *kspace_modify disp/auto yes* command.

A reasonable approach that combines the upsides of both methods is to make the first run using the *kspace_modify force/disp/real* and *kspace_modify force/disp/kspace* commands, write down the PPPM parameters from the output, and specify these parameters using the second approach in subsequent runs (which have the same composition, force field, and approximately the same volume).

Concerning the performance of the pppm/disp there are two more things to consider. The first is that when using the pppm/disp, the cutoff parameter does no longer affect the accuracy of the simulation (subject to that gewald/disp is adjusted when changing the cutoff). The performance can thus be increased by examining different values for the cutoff parameter. A lower bound for the cutoff is only set by the truncation error of the repulsive term of pair potentials.

The second is that the mixing rule of the pair style has an impact on the computation time when using the pppm/disp. Fastest computations are achieved when using the geometric mixing rule. Using the arithmetic mixing rule substantially increases the computational cost. The computational overhead can be reduced using the *kspace_modify mix/disp geom* and *kspace_modify splittol* commands. The first command simply enforces geometric mixing of the dispersion coefficients in kspace computations. This introduces some error in the computations but will also significantly speed-up the simulations. The second keyword sets the accuracy with which the dispersion coefficients are approximated using a matrix factorization approach. This may result in better accuracy then using the first command, but will usually also not provide an equally good increase of efficiency.

Finally, pppm/disp can also be used when no mixing rules apply. This can be achieved using the *kspace_modify mix/disp none* command. Note that the code does not check automatically whether any mixing rule is fulfilled. If mixing rules do not apply, the user will have to specify this command explicitly.

8.4 Analysis howto

8.4.1 Output from LAMMPS (thermo, dumps, computes, fixes, variables)

There are four basic kinds of LAMMPS output:

- *Thermodynamic output*, which is a list of quantities printed every few timesteps to the screen and logfile.
- *Dump files*, which contain snapshots of atoms and various per-atom values and are written at a specified frequency.
- Certain fixes can output user-specified quantities to files: *fix ave/time* for time averaging, *fix ave/chunk* for spatial or other averaging, and *fix print* for single-line output of *variables*. Fix print can also output to the screen.

- *Restart files*.

A simulation prints one set of thermodynamic output and (optionally) restart files. It can generate any number of dump files and fix output files, depending on what *dump* and *fix* commands you specify.

As discussed below, LAMMPS gives you a variety of ways to determine what quantities are computed and printed when the thermodynamics, dump, or fix commands listed above perform output. Throughout this discussion, note that users can also *add their own computes and fixes to LAMMPS* which can then generate values that can then be output with these commands.

The following sub-sections discuss different LAMMPS command related to output and the kind of data they operate on and produce:

- *Global/per-atom/local data*
- *Scalar/vector/array data*
- *Thermodynamic output*
- *Dump file output*
- *Fixes that write output files*
- *Computes that process output quantities*
- *Fixes that process output quantities*
- *Computes that generate values to output*
- *Fixes that generate values to output*
- *Variables that generate values to output*
- *Summary table of output options and data flow between commands*

Global/per-atom/local data

Various output-related commands work with three different styles of data: global, per-atom, or local. A global datum is one or more system-wide values, e.g. the temperature of the system. A per-atom datum is one or more values per atom, e.g. the kinetic energy of each atom. Local datums are calculated by each processor based on the atoms it owns, but there may be zero or more per atom, e.g. a list of bond distances.

Scalar/vector/array data

Global, per-atom, and local datums can each come in three kinds: a single scalar value, a vector of values, or a 2d array of values. The doc page for a "compute" or "fix" or "variable" that generates data will specify both the style and kind of data it produces, e.g. a per-atom vector.

When a quantity is accessed, as in many of the output commands discussed below, it can be referenced via the following bracket notation, where ID in this case is the ID of a compute. The leading "c_" would be replaced by "f_" for a fix, or "v_" for a variable:

c_ID	entire scalar, vector, or array
c_ID[I]	one element of vector, one column of array
c_ID[I][J]	one element of array

In other words, using one bracket reduces the dimension of the data once (vector -> scalar, array -> vector). Using two brackets reduces the dimension twice (array -> scalar). Thus a command that uses scalar values as input can typically also process elements of a vector or array.

Thermodynamic output

The frequency and format of thermodynamic output is set by the *thermo*, *thermo_style*, and *thermo_modify* commands. The *thermo_style* command also specifies what values are calculated and written out. Pre-defined keywords can be specified (e.g. press, etotal, etc). Three additional kinds of keywords can also be specified (c_ID, f_ID, v_name), where a *compute* or *fix* or *variable* provides the value to be output. In each case, the compute, fix, or variable must generate global values for input to the *thermo_style custom* command.

Note that thermodynamic output values can be "extensive" or "intensive". The former scale with the number of atoms in the system (e.g. total energy), the latter do not (e.g. temperature). The setting for *thermo_modify norm* determines whether extensive quantities are normalized or not. Computes and fixes produce either extensive or intensive values; see their individual doc pages for details. *Equal-style variables* produce only intensive values; you can include a division by "natoms" in the formula if desired, to make an extensive calculation produce an intensive result.

Dump file output

Dump file output is specified by the *dump* and *dump_modify* commands. There are several pre-defined formats (dump atom, dump xtc, etc).

There is also a *dump custom* format where the user specifies what values are output with each atom. Pre-defined atom attributes can be specified (id, x, fx, etc). Three additional kinds of keywords can also be specified (c_ID, f_ID, v_name), where a *compute* or *fix* or *variable* provides the values to be output. In each case, the compute, fix, or variable must generate per-atom values for input to the *dump custom* command.

There is also a *dump local* format where the user specifies what local values to output. A pre-defined index keyword can be specified to enumerate the local values. Two additional kinds of keywords can also be specified (c_ID, f_ID), where a *compute* or *fix* or *variable* provides the values to be output. In each case, the compute or fix must generate local values for input to the *dump local* command.

Fixes that write output files

Several fixes take various quantities as input and can write output files: *fix ave/time*, *fix ave/chunk*, *fix ave/histo*, *fix ave/correlate*, and *fix print*.

The *fix ave/time* command enables direct output to a file and/or time-averaging of global scalars or vectors. The user specifies one or more quantities as input. These can be global *compute* values, global *fix* values, or *variables* of any style except the atom style which produces per-atom values. Since a variable can refer to keywords used by the *thermo_style custom* command (like temp or press) and individual per-atom values, a wide variety of quantities can be time averaged and/or output in this way. If the inputs are one or more scalar values, then the fix generate a global scalar or vector of output. If the inputs are one or more vector values, then the fix generates a global vector or array of output. The time-averaged output of this fix can also be used as input to other output commands.

The *fix ave/chunk* command enables direct output to a file of chunk-averaged per-atom quantities like those output in dump files. Chunks can represent spatial bins or other collections of atoms, e.g. individual molecules. The per-atom quantities can be atom density (mass or number) or atom attributes such as position, velocity, force. They can also be per-atom quantities calculated by a *compute*, by a *fix*, or by an atom-style *variable*. The chunk-averaged output of this fix can also be used as input to other output commands.

The *fix ave/histo* command enables direct output to a file of histogrammed quantities, which can be global or per-atom or local quantities. The histogram output of this fix can also be used as input to other output commands.

The *fix ave/correlate* command enables direct output to a file of time-correlated quantities, which can be global values. The correlation matrix output of this fix can also be used as input to other output commands.

The *fix print* command can generate a line of output written to the screen and log file or to a separate file, periodically during a running simulation. The line can contain one or more *variable* values for any style variable except the

vector or atom styles). As explained above, variables themselves can contain references to global values generated by *thermodynamic keywords*, *computes*, *fixes*, or other *variables*, or to per-atom values for a specific atom. Thus the *fix print* command is a means to output a wide variety of quantities separate from normal thermodynamic or dump file output.

Computes that process output quantities

The *compute reduce* and *compute reduce/region* commands take one or more per-atom or local vector quantities as inputs and "reduce" them (sum, min, max, ave) to scalar quantities. These are produced as output values which can be used as input to other output commands.

The *compute slice* command take one or more global vector or array quantities as inputs and extracts a subset of their values to create a new vector or array. These are produced as output values which can be used as input to other output commands.

The *compute property/atom* command takes a list of one or more pre-defined atom attributes (id, x, fx, etc) and stores the values in a per-atom vector or array. These are produced as output values which can be used as input to other output commands. The list of atom attributes is the same as for the *dump custom* command.

The *compute property/local* command takes a list of one or more pre-defined local attributes (bond info, angle info, etc) and stores the values in a local vector or array. These are produced as output values which can be used as input to other output commands.

Fixes that process output quantities

The *fix vector* command can create global vectors as output from global scalars as input, accumulating them one element at a time.

The *fix ave/atom* command performs time-averaging of per-atom vectors. The per-atom quantities can be atom attributes such as position, velocity, force. They can also be per-atom quantities calculated by a *compute*, by a *fix*, or by an atom-style *variable*. The time-averaged per-atom output of this fix can be used as input to other output commands.

The *fix store/state* command can archive one or more per-atom attributes at a particular time, so that the old values can be used in a future calculation or output. The list of atom attributes is the same as for the *dump custom* command, including per-atom quantities calculated by a *compute*, by a *fix*, or by an atom-style *variable*. The output of this fix can be used as input to other output commands.

Computes that generate values to output

Every *compute* in LAMMPS produces either global or per-atom or local values. The values can be scalars or vectors or arrays of data. These values can be output using the other commands described in this section. The doc page for each compute command describes what it produces. Computes that produce per-atom or local values have the word "atom" or "local" in their style name. Computes without the word "atom" or "local" produce global values.

Fixes that generate values to output

Some *fixes* in LAMMPS produces either global or per-atom or local values which can be accessed by other commands. The values can be scalars or vectors or arrays of data. These values can be output using the other commands described in this section. The doc page for each fix command tells whether it produces any output quantities and describes them.

Variables that generate values to output

Variables defined in an input script can store one or more strings. But equal-style, vector-style, and atom-style or atomfile-style variables generate a global scalar value, global vector or values, or a per-atom vector, respectively, when accessed. The formulas used to define these variables can contain references to the thermodynamic keywords and to global and per-atom data generated by computes, fixes, and other variables. The values generated by variables can be used as input to and thus output by the other commands described in this section.

Summary table of output options and data flow between commands

This table summarizes the various commands that can be used for generating output from LAMMPS. Each command produces output data of some kind and/or writes data to a file. Most of the commands can take data from other commands as input. Thus you can link many of these commands together in pipeline form, where data produced by one command is used as input to another command and eventually written to the screen or to a file. Note that to hook two commands together the output and input data types must match, e.g. global/per-atom/local data and scalar/vector/array data.

Also note that, as described above, when a command takes a scalar as input, that could be an element of a vector or array. Likewise a vector input could be a column of an array.

Command	Input	Output
thermo_style custom	global scalars	screen, log file
dump custom	per-atom vectors	dump file
dump local	local vectors	dump file
fix print	global scalar from variable	screen, file
print	global scalar from variable	screen
computes	N/A	global/per-atom/local scalar/vector/array
fixes	N/A	global/per-atom/local scalar/vector/array
variables	global scalars and vectors, per-atom vectors	global scalar and vector, per-atom vector
compute reduce	per-atom/local vectors	global scalar/vector
compute slice	global vectors/arrays	global vector/array
compute property/atom	per-atom vectors	per-atom vector/array
compute property/local	local vectors	local vector/array
fix vector	global scalars	global vector
fix ave/atom	per-atom vectors	per-atom vector/array
fix ave/time	global scalars/vectors	global scalar/vector/array, file
fix ave/chunk	per-atom vectors	global array, file
fix ave/histo	global/per-atom/local scalars and vectors	global array, file
fix ave/correlate	global scalars	global array, file
fix store/state	per-atom vectors	per-atom vector/array

8.4.2 Use chunks to calculate system properties

In LAMMS, "chunks" are collections of atoms, as defined by the *compute chunk/atom* command, which assigns each atom to a chunk ID (or to no chunk at all). The number of chunks and the assignment of chunk IDs to atoms can be static or change over time. Examples of "chunks" are molecules or spatial bins or atoms with similar values (e.g. coordination number or potential energy).

The per-atom chunk IDs can be used as input to two other kinds of commands, to calculate various properties of a system:

- *fix ave/chunk*
- any of the *compute */chunk* commands

Here a brief overview for each of the 4 kinds of chunk-related commands is provided. Then some examples are given of how to compute different properties with chunk commands.

Compute chunk/atom command:

This compute can assign atoms to chunks of various styles. Only atoms in the specified group and optional specified region are assigned to a chunk. Here are some possible chunk definitions:

atoms in same molecule	chunk ID = molecule ID
atoms of same atom type	chunk ID = atom type
all atoms with same atom property (charge, radius, etc)	chunk ID = output of compute property/atom
atoms in same cluster	chunk ID = output of *compute cluster/atom* command
atoms in same spatial bin	chunk ID = bin ID
atoms in same rigid body	chunk ID = molecule ID used to define rigid bodies
atoms with similar potential energy	chunk ID = output of *compute pe/atom*
atoms with same local defect structure	chunk ID = output of *compute centro/atom* or *compute coord/atom* command

Note that chunk IDs are integer values, so for atom properties or computes that produce a floating point value, they will be truncated to an integer. You could also use the compute in a variable that scales the floating point value to spread it across multiple integers.

Spatial bins can be of various kinds, e.g. 1d bins = slabs, 2d bins = pencils, 3d bins = boxes, spherical bins, cylindrical bins.

This compute also calculates the number of chunks *Nchunk*, which is used by other commands to tally per-chunk data. *Nchunk* can be a static value or change over time (e.g. the number of clusters). The chunk ID for an individual atom can also be static (e.g. a molecule ID), or dynamic (e.g. what spatial bin an atom is in as it moves).

Note that this compute allows the per-atom output of other *computes*, *fixes*, and *variables* to be used to define chunk IDs for each atom. This means you can write your own compute or fix to output a per-atom quantity to use as chunk ID. See the *Modify* doc pages for info on how to do this. You can also define a *per-atom variable* in the input script that uses a formula to generate a chunk ID for each atom.

Fix ave/chunk command:

This fix takes the ID of a *compute chunk/atom* command as input. For each chunk, it then sums one or more specified per-atom values over the atoms in each chunk. The per-atom values can be any atom property, such as velocity, force, charge, potential energy, kinetic energy, stress, etc. Additional keywords are defined for per-chunk properties like density and temperature. More generally any per-atom value generated by other *computes*, *fixes*, and *per-atom variables*, can be summed over atoms in each chunk.

Similar to other averaging fixes, this fix allows the summed per-chunk values to be time-averaged in various ways, and output to a file. The fix produces a global array as output with one row of values per chunk.

Compute */chunk commands:

The following computes operate on chunks of atoms to produce per-chunk values. Any compute whose style name ends in "/chunk" is in this category:

- *compute com/chunk*
- *compute gyration/chunk*
- *compute inertia/chunk*
- *compute msd/chunk*
- *compute property/chunk*
- *compute temp/chunk*
- *compute torque/chunk*
- *compute vcm/chunk*

They each take the ID of a *compute chunk/atom* command as input. As their names indicate, they calculate the center-of-mass, radius of gyration, moments of inertia, mean-squared displacement, temperature, torque, and velocity of center-of-mass for each chunk of atoms. The *compute property/chunk* command can tally the count of atoms in each chunk and extract other per-chunk properties.

The reason these various calculations are not part of the *fix ave/chunk command*, is that each requires a more complicated operation than simply summing and averaging over per-atom values in each chunk. For example, many of them require calculation of a center of mass, which requires summing mass*position over the atoms and then dividing by summed mass.

All of these computes produce a global vector or global array as output, wih one or more values per chunk. The output can be used in various ways:

- As input to the *fix ave/time* command, which can write the values to a file and optionally time average them.
- As input to the *fix ave/histo* command to histogram values across chunks. E.g. a histogram of cluster sizes or molecule diffusion rates.
- As input to special functions of *equal-style variables*, like sum() and max() and ave(). E.g. to find the largest cluster or fastest diffusing molecule or average radius-of-gyration of a set of molecules (chunks).

Other chunk commands:

- *compute chunk/spread/atom*
- *compute reduce/chunk*

The *compute chunk/spread/atom* command spreads per-chunk values to each atom in the chunk, producing per-atom values as its output. This can be useful for outputting per-chunk values to a per-atom *dump file*. Or for using an atom's associated chunk value in an *atom-style variable*. Or as input to the *fix ave/chunk* command to spatially average per-chunk values calculated by a per-chunk compute.

The *compute reduce/chunk* command reduces a peratom value across the atoms in each chunk to produce a value per chunk. When used with the *compute chunk/spread/atom* command it can create peratom values that induce a new set of chunks with a second *compute chunk/atom* command.

Example calculations with chunks

Here are examples using chunk commands to calculate various properties:

(1) Average velocity in each of 1000 2d spatial bins:

```
compute cc1 all chunk/atom bin/2d x 0.0 0.1 y lower 0.01 units reduced
fix 1 all ave/chunk 100 10 1000 cc1 vx vy file tmp.out
```

(2) Temperature in each spatial bin, after subtracting a flow velocity:

```
compute cc1 all chunk/atom bin/2d x 0.0 0.1 y lower 0.1 units reduced
compute vbias all temp/profile 1 0 0 y 10
fix 1 all ave/chunk 100 10 1000 cc1 temp bias vbias file tmp.out
```

(3) Center of mass of each molecule:

```
compute cc1 all chunk/atom molecule
compute myChunk all com/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk[*] file tmp.out mode vector
```

(4) Total force on each molecule and ave/max across all molecules:

```
compute cc1 all chunk/atom molecule
fix 1 all ave/chunk 1000 1 1000 cc1 fx fy fz file tmp.out
variable xave equal ave(f_1[2])
variable xmax equal max(f_1[2])
thermo 1000
thermo_style custom step temp v_xave v_xmax
```

(5) Histogram of cluster sizes:

```
compute cluster all cluster/atom 1.0
compute cc1 all chunk/atom c_cluster compress yes
compute size all property/chunk cc1 count
fix 1 all ave/histo 100 1 100 0 20 20 c_size mode vector ave running beyond ignore␣
↪file tmp.histo
```

(6) An example for using a per-chunk value to apply per-atom forces to compress individual polymer chains (molecules) in a mixture, is explained on the *compute chunk/spread/atom* command doc page.

(7) An example for using one set of per-chunk values for molecule chunks, to create a 2nd set of micelle-scale chunks (clustered molecules, due to hydrophobicity), is explained on the *compute chunk/reduce* command doc page.

(8) An example for using one set of per-chunk values (dipole moment vectors) for molecule chunks, spreading the values to each atom in each chunk, then defining a second set of chunks as spatial bins, and using the *fix ave/chunk* command to calculate an average dipole moment vector for each bin. This example is explained on the *compute chunk/spread/atom* command doc page.

8.4.3 Calculate temperature

Temperature is computed as kinetic energy divided by some number of degrees of freedom (and the Boltzmann constant). Since kinetic energy is a function of particle velocity, there is often a need to distinguish between a particle's advection velocity (due to some aggregate motion of particles) and its thermal velocity. The sum of the two is the particle's total velocity, but the latter is often what is wanted to compute a temperature.

LAMMPS has several options for computing temperatures, any of which can be used in *thermostatting* and *barostatting*. These *compute commands* calculate temperature:

- *compute temp*
- *compute temp/sphere*
- *compute temp/asphere*
- *compute temp/com*
- *compute temp/deform*
- *compute temp/partial*
- *compute temp/profile*
- *compute temp/ramp*
- *compute temp/region*

All but the first 3 calculate velocity biases directly (e.g. advection velocities) that are removed when computing the thermal temperature. *Compute temp/sphere* and *compute temp/asphere* compute kinetic energy for finite-size particles that includes rotational degrees of freedom. They both allow for velocity biases indirectly, via an optional extra argument which is another temperature compute that subtracts a velocity bias. This allows the translational velocity of spherical or aspherical particles to be adjusted in prescribed ways.

8.4.4 Calculate elastic constants

Elastic constants characterize the stiffness of a material. The formal definition is provided by the linear relation that holds between the stress and strain tensors in the limit of infinitesimal deformation. In tensor notation, this is expressed as s_ij = C_ijkl * e_kl, where the repeated indices imply summation. s_ij are the elements of the symmetric stress tensor. e_kl are the elements of the symmetric strain tensor. C_ijkl are the elements of the fourth rank tensor of elastic constants. In three dimensions, this tensor has 3^4=81 elements. Using Voigt notation, the tensor can be written as a 6x6 matrix, where C_ij is now the derivative of s_i w.r.t. e_j. Because s_i is itself a derivative w.r.t. e_i, it follows that C_ij is also symmetric, with at most 7*6/2 = 21 distinct elements.

At zero temperature, it is easy to estimate these derivatives by deforming the simulation box in one of the six directions using the *change_box* command and measuring the change in the stress tensor. A general-purpose script that does this is given in the examples/elastic directory described on the *Examples* doc page.

Calculating elastic constants at finite temperature is more challenging, because it is necessary to run a simulation that performs time averages of differential properties. One way to do this is to measure the change in average stress tensor in an NVT simulations when the cell volume undergoes a finite deformation. In order to balance the systematic and statistical errors in this method, the magnitude of the deformation must be chosen judiciously, and care must be taken to fully equilibrate the deformed cell before sampling the stress tensor. Another approach is to sample the triclinic

cell fluctuations that occur in an NPT simulation. This method can also be slow to converge and requires careful post-processing *(Shinoda)*

(Shinoda) Shinoda, Shiga, and Mikami, Phys Rev B, 69, 134103 (2004).

8.4.5 Calculate thermal conductivity

The thermal conductivity kappa of a material can be measured in at least 4 ways using various options in LAMMPS. See the examples/KAPPA directory for scripts that implement the 4 methods discussed here for a simple Lennard-Jones fluid model. Also, see the *Howto viscosity* doc page for an analogous discussion for viscosity.

The thermal conductivity tensor kappa is a measure of the propensity of a material to transmit heat energy in a diffusive manner as given by Fourier's law

J = -kappa grad(T)

where J is the heat flux in units of energy per area per time and grad(T) is the spatial gradient of temperature. The thermal conductivity thus has units of energy per distance per time per degree K and is often approximated as an isotropic quantity, i.e. as a scalar.

The first method is to setup two thermostatted regions at opposite ends of a simulation box, or one in the middle and one at the end of a periodic box. By holding the two regions at different temperatures with a *thermostatting fix*, the energy added to the hot region should equal the energy subtracted from the cold region and be proportional to the heat flux moving between the regions. See the papers by *Ikeshoji and Hafskjold* and *Wirnsberger et al* for details of this idea. Note that thermostatting fixes such as *fix nvt*, *fix langevin*, and *fix temp/rescale* store the cumulative energy they add/subtract.

Alternatively, as a second method, the *fix heat* or *fix ehex* commands can be used in place of thermostats on each of two regions to add/subtract specified amounts of energy to both regions. In both cases, the resulting temperatures of the two regions can be monitored with the "compute temp/region" command and the temperature profile of the intermediate region can be monitored with the *fix ave/chunk* and *compute ke/atom* commands.

The third method is to perform a reverse non-equilibrium MD simulation using the *fix thermal/conductivity* command which implements the rNEMD algorithm of Muller-Plathe. Kinetic energy is swapped between atoms in two different layers of the simulation box. This induces a temperature gradient between the two layers which can be monitored with the *fix ave/chunk* and *compute ke/atom* commands. The fix tallies the cumulative energy transfer that it performs. See the *fix thermal/conductivity* command for details.

The fourth method is based on the Green-Kubo (GK) formula which relates the ensemble average of the auto-correlation of the heat flux to kappa. The heat flux can be calculated from the fluctuations of per-atom potential and kinetic energies and per-atom stress tensor in a steady-state equilibrated simulation. This is in contrast to the two preceding non-equilibrium methods, where energy flows continuously between hot and cold regions of the simulation box.

The *compute heat/flux* command can calculate the needed heat flux and describes how to implement the Green_Kubo formalism using additional LAMMPS commands, such as the *fix ave/correlate* command to calculate the needed auto-correlation. See the doc page for the *compute heat/flux* command for an example input script that calculates the thermal conductivity of solid Ar via the GK formalism.

(Ikeshoji) Ikeshoji and Hafskjold, Molecular Physics, 81, 251-261 (1994).

(Wirnsberger) Wirnsberger, Frenkel, and Dellago, J Chem Phys, 143, 124104 (2015).

8.4.6 Calculate viscosity

The shear viscosity eta of a fluid can be measured in at least 5 ways using various options in LAMMPS. See the examples/VISCOSITY directory for scripts that implement the 5 methods discussed here for a simple Lennard-Jones fluid model. Also, see the *Howto kappa* doc page for an analogous discussion for thermal conductivity.

Eta is a measure of the propensity of a fluid to transmit momentum in a direction perpendicular to the direction of velocity or momentum flow. Alternatively it is the resistance the fluid has to being sheared. It is given by

J = -eta grad(Vstream)

where J is the momentum flux in units of momentum per area per time. and grad(Vstream) is the spatial gradient of the velocity of the fluid moving in another direction, normal to the area through which the momentum flows. Viscosity thus has units of pressure-time.

The first method is to perform a non-equilibrium MD (NEMD) simulation by shearing the simulation box via the *fix deform* command, and using the *fix nvt/sllod* command to thermostat the fluid via the SLLOD equations of motion. Alternatively, as a second method, one or more moving walls can be used to shear the fluid in between them, again with some kind of thermostat that modifies only the thermal (non-shearing) components of velocity to prevent the fluid from heating up.

Note: A recent (2017) book by *(Daivis and Todd)* discusses use of the SLLOD method and non-equilibrium MD (NEMD) thermostatting generally, for both simple and complex fluids, e.g. molecular systems. The latter can be tricky to do correctly.

In both cases, the velocity profile setup in the fluid by this procedure can be monitored by the *fix ave/chunk* command, which determines grad(Vstream) in the equation above. E.g. the derivative in the y-direction of the Vx component of fluid motion or grad(Vstream) = dVx/dy. The Pxy off-diagonal component of the pressure or stress tensor, as calculated by the *compute pressure* command, can also be monitored, which is the J term in the equation above. See the *Howto nemd* doc page for details on NEMD simulations.

The third method is to perform a reverse non-equilibrium MD simulation using the *fix viscosity* command which implements the rNEMD algorithm of Muller-Plathe. Momentum in one dimension is swapped between atoms in two different layers of the simulation box in a different dimension. This induces a velocity gradient which can be monitored with the *fix ave/chunk* command. The fix tallies the cumulative momentum transfer that it performs. See the *fix viscosity* command for details.

The fourth method is based on the Green-Kubo (GK) formula which relates the ensemble average of the auto-correlation of the stress/pressure tensor to eta. This can be done in a fully equilibrated simulation which is in contrast to the two preceding non-equilibrium methods, where momentum flows continuously through the simulation box.

Here is an example input script that calculates the viscosity of liquid Ar via the GK formalism:

```
# Sample LAMMPS input script for viscosity of liquid Ar

units       real
variable    T equal 86.4956
variable    V equal vol
variable    dt equal 4.0
variable    p equal 400     # correlation length
variable    s equal 5       # sample interval
variable    d equal $p*$s   # dump interval

# convert from LAMMPS real units to SI

variable    kB equal 1.3806504e-23    # [J/K] Boltzmann
variable    atm2Pa equal 101325.0
```

(continues on next page)

(continued from previous page)

```
variable    A2m equal 1.0e-10
variable    fs2s equal 1.0e-15
variable    convert equal ${atm2Pa}*${atm2Pa}*${fs2s}*${A2m}*${A2m}*${A2m}

# setup problem

dimension    3
boundary     p p p
lattice      fcc 5.376 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1
region       box block 0 4 0 4 0 4
create_box   1 box
create_atoms 1 box
mass         1 39.948
pair_style   lj/cut 13.0
pair_coeff   * * 0.2381 3.405
timestep     ${dt}
thermo       $d

# equilibration and thermalization

velocity     all create $T 102486 mom yes rot yes dist gaussian
fix          NVT all nvt temp $T $T 10 drag 0.2
run          8000

# viscosity calculation, switch to NVE if desired

#unfix       NVT
#fix         NVE all nve

reset_timestep 0
variable     pxy equal pxy
variable     pxz equal pxz
variable     pyz equal pyz
fix          SS all ave/correlate $s $p $d &
             v_pxy v_pxz v_pyz type auto file S0St.dat ave running
variable     scale equal ${convert}/(${kB}*$T)*$V*$s*${dt}
variable     v11 equal trap(f_SS[3])*${scale}
variable     v22 equal trap(f_SS[4])*${scale}
variable     v33 equal trap(f_SS[5])*${scale}
thermo_style custom step temp press v_pxy v_pxz v_pyz v_v11 v_v22 v_v33
run          100000
variable     v equal (v_v11+v_v22+v_v33)/3.0
variable     ndens equal count(all)/vol
print        "average viscosity: $v [Pa.s] @ $T K, ${ndens} /A^3"
```

The fifth method is related to the above Green-Kubo method, but uses the Einstein formulation, analogous to the Einstein mean-square-displacement formulation for self-diffusivity. The time-integrated momentum fluxes play the role of Cartesian coordinates, whose mean-square displacement increases linearly with time at sufficiently long times.

(Daivis and Todd) Daivis and Todd, Nonequilibrium Molecular Dynamics (book), Cambridge University Press, https://doi.org/10.1017/9781139017848, (2017).

8.4.7 Calculate diffusion coefficients

The diffusion coefficient D of a material can be measured in at least 2 ways using various options in LAMMPS. See the examples/DIFFUSE directory for scripts that implement the 2 methods discussed here for a simple Lennard-Jones fluid model.

The first method is to measure the mean-squared displacement (MSD) of the system, via the *compute msd* command. The slope of the MSD versus time is proportional to the diffusion coefficient. The instantaneous MSD values can be accumulated in a vector via the *fix vector* command, and a line fit to the vector to compute its slope via the *variable slope* function, and thus extract D.

The second method is to measure the velocity auto-correlation function (VACF) of the system, via the *compute vacf* command. The time-integral of the VACF is proportional to the diffusion coefficient. The instantaneous VACF values can be accumulated in a vector via the *fix vector* command, and time integrated via the *variable trap* function, and thus extract D.

8.5 Force fields howto

8.5.1 CHARMM, AMBER, COMPASS, and DREIDING force fields

A force field has 2 parts: the formulas that define it and the coefficients used for a particular system. Here we only discuss formulas implemented in LAMMPS that correspond to formulas commonly used in the CHARMM, AMBER, COMPASS, and DREIDING force fields. Setting coefficients is done either from special sections in an input data file via the *read_data* command or in the input script with commands like *pair_coeff* or *bond_coeff* and so on. See the *Tools* doc page for additional tools that can use CHARMM, AMBER, or Materials Studio generated files to assign force field coefficients and convert their output into LAMMPS input.

See *(MacKerell)* for a description of the CHARMM force field. See *(Cornell)* for a description of the AMBER force field. See *(Sun)* for a description of the COMPASS force field.

The interaction styles listed below compute force field formulas that are consistent with common options in CHARMM or AMBER. See each command's documentation for the formula it computes.

- *bond_style* harmonic
- *angle_style* charmm
- *dihedral_style* charmmfsh
- *dihedral_style* charmm
- *pair_style* lj/charmmfsw/coul/charmmfsh
- *pair_style* lj/charmmfsw/coul/long
- *pair_style* lj/charmm/coul/charmm
- *pair_style* lj/charmm/coul/charmm/implicit
- *pair_style* lj/charmm/coul/long
- *special_bonds* charmm
- *special_bonds* amber

Note: For CHARMM, newer *charmmfsw* or *charmmfsh* styles were released in March 2017. We recommend they be used instead of the older *charmm* styles. See discussion of the differences on the *pair charmm* and *dihedral charmm* doc pages.

COMPASS is a general force field for atomistic simulation of common organic molecules, inorganic small molecules, and polymers which was developed using ab initio and empirical parameterization techniques. See the *Tools* doc page for the msi2lmp tool for creating LAMMPS template input and data files from BIOVIA's Materials Studio files. Please note that the msi2lmp tool is very old and largely unmaintained, so it does not support all features of Materials Studio provided force field files, especially additions during the last decade. You should watch the output carefully and compare results, where possible. See *(Sun)* for a description of the COMPASS force field.

These interaction styles listed below compute force field formulas that are consistent with the COMPASS force field. See each command's documentation for the formula it computes.

- *bond_style* class2
- *angle_style* class2
- *dihedral_style* class2
- *improper_style* class2
- *pair_style* lj/class2
- *pair_style* lj/class2/coul/cut
- *pair_style* lj/class2/coul/long
- *special_bonds* lj/coul 0 0 1

DREIDING is a generic force field developed by the Goddard group at Caltech and is useful for predicting structures and dynamics of organic, biological and main-group inorganic molecules. The philosophy in DREIDING is to use general force constants and geometry parameters based on simple hybridization considerations, rather than individual force constants and geometric parameters that depend on the particular combinations of atoms involved in the bond, angle, or torsion terms. DREIDING has an *explicit hydrogen bond term* to describe interactions involving a hydrogen atom on very electronegative atoms (N, O, F).

See *(Mayo)* for a description of the DREIDING force field

The interaction styles listed below compute force field formulas that are consistent with the DREIDING force field. See each command's documentation for the formula it computes.

- *bond_style* harmonic
- *bond_style* morse
- *angle_style* harmonic
- *angle_style* cosine
- *angle_style* cosine/periodic
- *dihedral_style* charmm
- *improper_style* umbrella
- *pair_style* buck
- *pair_style* buck/coul/cut
- *pair_style* buck/coul/long
- *pair_style* lj/cut
- *pair_style* lj/cut/coul/cut
- *pair_style* lj/cut/coul/long
- *pair_style* hbond/dreiding/lj
- *pair_style* hbond/dreiding/morse

- *special_bonds* dreiding

(MacKerell) MacKerell, Bashford, Bellott, Dunbrack, Evanseck, Field, Fischer, Gao, Guo, Ha, et al, J Phys Chem, 102, 3586 (1998).

(Cornell) Cornell, Cieplak, Bayly, Gould, Merz, Ferguson, Spellmeyer, Fox, Caldwell, Kollman, JACS 117, 5179-5197 (1995).

(Sun) Sun, J. Phys. Chem. B, 102, 7338-7364 (1998).

(Mayo) Mayo, Olfason, Goddard III, J Phys Chem, 94, 8897-8909 (1990).

8.5.2 TIP3P water model

The TIP3P water model as implemented in CHARMM *(MacKerell)* specifies a 3-site rigid water molecule with charges and Lennard-Jones parameters assigned to each of the 3 atoms. In LAMMPS the *fix shake* command can be used to hold the two O-H bonds and the H-O-H angle rigid. A bond style of *harmonic* and an angle style of *harmonic* or *charmm* should also be used.

These are the additional parameters (in real units) to set for O and H atoms and the water molecule to run a rigid TIP3P-CHARMM model with a cutoff. The K values can be used if a flexible TIP3P model (without fix shake) is desired. If the LJ epsilon and sigma for HH and OH are set to 0.0, it corresponds to the original 1983 TIP3P model *(Jorgensen)*.

O mass = 15.9994
H mass = 1.008
O charge = -0.834
H charge = 0.417
LJ epsilon of OO = 0.1521
LJ sigma of OO = 3.1507
LJ epsilon of HH = 0.0460
LJ sigma of HH = 0.4000
LJ epsilon of OH = 0.0836
LJ sigma of OH = 1.7753
K of OH bond = 450
r0 of OH bond = 0.9572
K of HOH angle = 55
theta of HOH angle = 104.52

These are the parameters to use for TIP3P with a long-range Coulombic solver (e.g. Ewald or PPPM in LAMMPS), see *(Price)* for details:

O mass = 15.9994
H mass = 1.008
O charge = -0.830
H charge = 0.415
LJ epsilon of OO = 0.102

LJ sigma of OO = 3.188
LJ epsilon, sigma of OH, HH = 0.0
K of OH bond = 450
r0 of OH bond = 0.9572
K of HOH angle = 55
theta of HOH angle = 104.52

Wikipedia also has a nice article on water models.

(MacKerell) MacKerell, Bashford, Bellott, Dunbrack, Evanseck, Field, Fischer, Gao, Guo, Ha, et al, J Phys Chem, 102, 3586 (1998).

(Jorgensen) Jorgensen, Chandrasekhar, Madura, Impey, Klein, J Chem Phys, 79, 926 (1983).

(Price) Price and Brooks, J Chem Phys, 121, 10096 (2004).

8.5.3 TIP4P water model

The four-point TIP4P rigid water model extends the traditional three-point TIP3P model by adding an additional site, usually massless, where the charge associated with the oxygen atom is placed. This site M is located at a fixed distance away from the oxygen along the bisector of the HOH bond angle. A bond style of *harmonic* and an angle style of *harmonic* or *charmm* should also be used.

A TIP4P model is run with LAMMPS using either this command for a cutoff model:

pair_style lj/cut/tip4p/cut

or these two commands for a long-range model:

- *pair_style lj/cut/tip4p/long*
- *kspace_style pppm/tip4p*

For both models, the bond lengths and bond angles should be held fixed using the *fix shake* command.

These are the additional parameters (in real units) to set for O and H atoms and the water molecule to run a rigid TIP4P model with a cutoff *(Jorgensen)*. Note that the OM distance is specified in the *pair_style* command, not as part of the pair coefficients.

O mass = 15.9994
H mass = 1.008
O charge = -1.040
H charge = 0.520
r0 of OH bond = 0.9572
theta of HOH angle = 104.52
OM distance = 0.15
LJ epsilon of O-O = 0.1550
LJ sigma of O-O = 3.1536
LJ epsilon, sigma of OH, HH = 0.0
Coulombic cutoff = 8.5

For the TIP4/Ice model (J Chem Phys, 122, 234511 (2005); http://dx.doi.org/10.1063/1.1931662) these values can be used:

O mass = 15.9994
H mass = 1.008
O charge = -1.1794
H charge = 0.5897
r0 of OH bond = 0.9572
theta of HOH angle = 104.52
OM distance = 0.1577
LJ epsilon of O-O = 0.21084
LJ sigma of O-O = 3.1668
LJ epsilon, sigma of OH, HH = 0.0
Coulombic cutoff = 8.5

For the TIP4P/2005 model (J Chem Phys, 123, 234505 (2005); http://dx.doi.org/10.1063/1.2121687), these values can be used:

O mass = 15.9994
H mass = 1.008
O charge = -1.1128
H charge = 0.5564
r0 of OH bond = 0.9572
theta of HOH angle = 104.52
OM distance = 0.1546
LJ epsilon of O-O = 0.1852
LJ sigma of O-O = 3.1589
LJ epsilon, sigma of OH, HH = 0.0
Coulombic cutoff = 8.5

These are the parameters to use for TIP4P with a long-range Coulombic solver (e.g. Ewald or PPPM in LAMMPS):

O mass = 15.9994
H mass = 1.008
O charge = -1.0484
H charge = 0.5242
r0 of OH bond = 0.9572
theta of HOH angle = 104.52
OM distance = 0.1250
LJ epsilon of O-O = 0.16275
LJ sigma of O-O = 3.16435
LJ epsilon, sigma of OH, HH = 0.0

Note that the when using the TIP4P pair style, the neighbor list cutoff for Coulomb interactions is effectively extended by a distance 2 * (OM distance), to account for the offset distance of the fictitious charges on O atoms in water molecules. Thus it is typically best in an efficiency sense to use a LJ cutoff >= Coulomb cutoff + 2*(OM distance), to shrink the size of the neighbor list. This leads to slightly larger cost for the long-range calculation, so you can test the trade-off for your model. The OM distance and the LJ and Coulombic cutoffs are set in the *pair_style lj/cut/tip4p/long* command.

Wikipedia also has a nice article on water models.

(Jorgensen) Jorgensen, Chandrasekhar, Madura, Impey, Klein, J Chem Phys, 79, 926 (1983).

8.5.4 SPC water model

The SPC water model specifies a 3-site rigid water molecule with charges and Lennard-Jones parameters assigned to each of the 3 atoms. In LAMMPS the *fix shake* command can be used to hold the two O-H bonds and the H-O-H angle rigid. A bond style of *harmonic* and an angle style of *harmonic* or *charmm* should also be used.

These are the additional parameters (in real units) to set for O and H atoms and the water molecule to run a rigid SPC model.

O mass = 15.9994
H mass = 1.008
O charge = -0.820
H charge = 0.410
LJ epsilon of OO = 0.1553
LJ sigma of OO = 3.166
LJ epsilon, sigma of OH, HH = 0.0
r0 of OH bond = 1.0
theta of HOH angle = 109.47

Note that as originally proposed, the SPC model was run with a 9 Angstrom cutoff for both LJ and Coulombic terms. It can also be used with long-range Coulombics (Ewald or PPPM in LAMMPS), without changing any of the parameters above, though it becomes a different model in that mode of usage.

The SPC/E (extended) water model is the same, except the partial charge assignments change:

O charge = -0.8476
H charge = 0.4238

See the *(Berendsen)* reference for more details on both the SPC and SPC/E models.

Wikipedia also has a nice article on water models.

(Berendsen) Berendsen, Grigera, Straatsma, J Phys Chem, 91, 6269-6271 (1987).

8.6 Packages howto

8.6.1 Finite-size spherical and aspherical particles

Typical MD models treat atoms or particles as point masses. Sometimes it is desirable to have a model with finite-size particles such as spheroids or ellipsoids or generalized aspherical bodies. The difference is that such particles have a moment of inertia, rotational energy, and angular momentum. Rotation is induced by torque coming from interactions with other particles.

LAMMPS has several options for running simulations with these kinds of particles. The following aspects are discussed in turn:

- atom styles
- pair potentials
- time integration
- computes, thermodynamics, and dump output
- rigid bodies composed of finite-size particles

Example input scripts for these kinds of models are in the body, colloid, dipole, ellipse, line, peri, pour, and tri directories of the *examples directory* in the LAMMPS distribution.

Atom styles

There are several *atom styles* that allow for definition of finite-size particles: sphere, dipole, ellipsoid, line, tri, peri, and body.

The sphere style defines particles that are spheroids and each particle can have a unique diameter and mass (or density). These particles store an angular velocity (omega) and can be acted upon by torque. The "set" command can be used to modify the diameter and mass of individual particles, after then are created.

The dipole style does not actually define finite-size particles, but is often used in conjunction with spherical particles, via a command like

```
atom_style hybrid sphere dipole
```

This is because when dipoles interact with each other, they induce torques, and a particle must be finite-size (i.e. have a moment of inertia) in order to respond and rotate. See the *atom_style dipole* command for details. The "set" command can be used to modify the orientation and length of the dipole moment of individual particles, after then are created.

The ellipsoid style defines particles that are ellipsoids and thus can be aspherical. Each particle has a shape, specified by 3 diameters, and mass (or density). These particles store an angular momentum and their orientation (quaternion), and can be acted upon by torque. They do not store an angular velocity (omega), which can be in a different direction than angular momentum, rather they compute it as needed. The "set" command can be used to modify the diameter, orientation, and mass of individual particles, after then are created. It also has a brief explanation of what quaternions are.

The line style defines line segment particles with two end points and a mass (or density). They can be used in 2d simulations, and they can be joined together to form rigid bodies which represent arbitrary polygons.

The tri style defines triangular particles with three corner points and a mass (or density). They can be used in 3d simulations, and they can be joined together to form rigid bodies which represent arbitrary particles with a triangulated surface.

The peri style is used with *Peridynamic models* and defines particles as having a volume, that is used internally in the *pair_style peri* potentials.

The body style allows for definition of particles which can represent complex entities, such as surface meshes of discrete points, collections of sub-particles, deformable objects, etc. The body style is discussed in more detail on the *Howto body* doc page.

Note that if one of these atom styles is used (or multiple styles via the *atom_style hybrid* command), not all particles in the system are required to be finite-size or aspherical.

For example, in the ellipsoid style, if the 3 shape parameters are set to the same value, the particle will be a sphere rather than an ellipsoid. If the 3 shape parameters are all set to 0.0 or if the diameter is set to 0.0, it will be a point particle. In the line or tri style, if the lineflag or triflag is specified as 0, then it will be a point particle.

Some of the pair styles used to compute pairwise interactions between finite-size particles also compute the correct interaction with point particles as well, e.g. the interaction between a point particle and a finite-size particle or between two point particles. If necessary, *pair_style hybrid* can be used to insure the correct interactions are computed for the appropriate style of interactions. Likewise, using groups to partition particles (ellipsoids versus spheres versus point particles) will allow you to use the appropriate time integrators and temperature computations for each class of particles. See the doc pages for various commands for details.

Also note that for *2d simulations*, atom styles sphere and ellipsoid still use 3d particles, rather than as circular disks or ellipses. This means they have the same moment of inertia as the 3d object. When temperature is computed, the correct degrees of freedom are used for rotation in a 2d versus 3d system.

Pair potentials

When a system with finite-size particles is defined, the particles will only rotate and experience torque if the force field computes such interactions. These are the various *pair styles* that generate torque:

- *pair_style gran/history*
- *pair_style gran/hertzian*
- *pair_style gran/no_history*
- *pair_style dipole/cut*
- *pair_style gayberne*
- *pair_style resquared*
- *pair_style brownian*
- *pair_style lubricate*
- *pair_style line/lj*
- *pair_style tri/lj*
- *pair_style body/nparticle*

The granular pair styles are used with spherical particles. The dipole pair style is used with the dipole atom style, which could be applied to spherical or ellipsoidal particles. The GayBerne and REsquared potentials require ellipsoidal particles, though they will also work if the 3 shape parameters are the same (a sphere). The Brownian and lubrication potentials are used with spherical particles. The line, tri, and body potentials are used with line segment, triangular, and body particles respectively.

Time integration

There are several fixes that perform time integration on finite-size spherical particles, meaning the integrators update the rotational orientation and angular velocity or angular momentum of the particles:

- *fix nve/sphere*
- *fix nvt/sphere*
- *fix npt/sphere*

Likewise, there are 3 fixes that perform time integration on ellipsoidal particles:

- *fix nve/asphere*
- *fix nvt/asphere*
- *fix npt/asphere*

The advantage of these fixes is that those which thermostat the particles include the rotational degrees of freedom in the temperature calculation and thermostatting. The *fix langevin* command can also be used with its *omgea* or *angmom* options to thermostat the rotational degrees of freedom for spherical or ellipsoidal particles. Other thermostatting fixes only operate on the translational kinetic energy of finite-size particles.

These fixes perform constant NVE time integration on line segment, triangular, and body particles:

- *fix nve/line*
- *fix nve/tri*
- *fix nve/body*

Note that for mixtures of point and finite-size particles, these integration fixes can only be used with *groups* which contain finite-size particles.

Computes, thermodynamics, and dump output

There are several computes that calculate the temperature or rotational energy of spherical or ellipsoidal particles:

- *compute temp/sphere*
- *compute temp/asphere*
- *compute erotate/sphere*
- *compute erotate/asphere*

These include rotational degrees of freedom in their computation. If you wish the thermodynamic output of temperature or pressure to use one of these computes (e.g. for a system entirely composed of finite-size particles), then the compute can be defined and the *thermo_modify* command used. Note that by default thermodynamic quantities will be calculated with a temperature that only includes translational degrees of freedom. See the *thermo_style* command for details.

These commands can be used to output various attributes of finite-size particles:

- *dump custom*
- *compute property/atom*
- *dump local*
- *compute body/local*

Attributes include the dipole moment, the angular velocity, the angular momentum, the quaternion, the torque, the end-point and corner-point coordinates (for line and tri particles), and sub-particle attributes of body particles.

Rigid bodies composed of finite-size particles

The *fix rigid* command treats a collection of particles as a rigid body, computes its inertia tensor, sums the total force and torque on the rigid body each timestep due to forces on its constituent particles, and integrates the motion of the rigid body.

If any of the constituent particles of a rigid body are finite-size particles (spheres or ellipsoids or line segments or triangles), then their contribution to the inertia tensor of the body is different than if they were point particles. This means the rotational dynamics of the rigid body will be different. Thus a model of a dimer is different if the dimer consists of two point masses versus two spheroids, even if the two particles have the same mass. Finite-size particles that experience torque due to their interaction with other particles will also impart that torque to a rigid body they are part of.

See the "fix rigid" command for example of complex rigid-body models it is possible to define in LAMMPS.

Note that the *fix shake* command can also be used to treat 2, 3, or 4 particles as a rigid body, but it always assumes the particles are point masses.

Also note that body particles cannot be modeled with the *fix rigid* command. Body particles are treated by LAMMPS as single particles, though they can store internal state, such as a list of sub-particles. Individual body particles are typically treated as rigid bodies, and their motion integrated with a command like *fix nve/body*. Interactions between pairs of body particles are computed via a command like *pair_style body/nparticle*.

8.6.2 Granular models

Granular system are composed of spherical particles with a diameter, as opposed to point particles. This means they have an angular velocity and torque can be imparted to them to cause them to rotate.

To run a simulation of a granular model, you will want to use the following commands:

- *atom_style sphere*
- *fix nve/sphere*
- *fix gravity*

This compute

- *compute erotate/sphere*

calculates rotational kinetic energy which can be *output with thermodynamic info*.

Use one of these 3 pair potentials, which compute forces and torques between interacting pairs of particles:

- *pair_style* gran/history
- *pair_style* gran/no_history
- *pair_style* gran/hertzian

These commands implement fix options specific to granular systems:

- *fix freeze*
- *fix pour*
- *fix viscous*
- *fix wall/gran*

The fix style *freeze* zeroes both the force and torque of frozen atoms, and should be used for granular system instead of the fix style *setforce*.

For computational efficiency, you can eliminate needless pairwise computations between frozen atoms by using this command:

- *neigh_modify* exclude

Note: By default, for 2d systems, granular particles are still modeled as 3d spheres, not 2d discs (circles), meaning their moment of inertia will be the same as in 3d. If you wish to model granular particles in 2d as 2d discs, see the note on this topic on the *Howto 2d* doc page, where 2d simulations are discussed.

8.6.3 Body particles

Overview:

In LAMMPS, body particles are generalized finite-size particles. Individual body particles can represent complex entities, such as surface meshes of discrete points, collections of sub-particles, deformable objects, etc. Note that other kinds of finite-size spherical and aspherical particles are also supported by LAMMPS, such as spheres, ellipsoids, line segments, and triangles, but they are simpler entities that body particles. See the *Howto spherical* doc page for a general overview of all these particle types.

Body particles are used via the *atom_style body* command. It takes a body style as an argument. The current body styles supported by LAMMPS are as follows. The name in the first column is used as the *bstyle* argument for the *atom_style body* command.

nparticle	rigid body with N sub-particles
rounded/polygon	2d polygons with N vertices
rounded/polyhedron	3d polyhedra with N vertices, E edges and F faces

The body style determines what attributes are stored for each body and thus how they can be used to compute pairwise body/body or bond/non-body (point particle) interactions. More details of each style are described below.

More styles may be added in the future. See the *Modify body* doc page for details on how to add a new body style to the code.

When to use body particles:

You should not use body particles to model a rigid body made of simpler particles (e.g. point, sphere, ellipsoid, line segment, triangular particles), if the interaction between pairs of rigid bodies is just the summation of pairwise interactions between the simpler particles. LAMMPS already supports this kind of model via the *fix rigid* command. Any of the numerous pair styles that compute interactions between simpler particles can be used. The *fix rigid* command time integrates the motion of the rigid bodies. All of the standard LAMMPS commands for thermostatting, adding constraints, performing output, etc will operate as expected on the simple particles.

By contrast, when body particles are used, LAMMPS treats an entire body as a single particle for purposes of computing pairwise interactions, building neighbor lists, migrating particles between processors, output of particles to a dump file, etc. This means that interactions between pairs of bodies or between a body and non-body (point) particle need to be encoded in an appropriate pair style. If such a pair style were to mimic the *fix rigid* model, it would need to loop over the entire collection of interactions between pairs of simple particles within the two bodies, each time a single body/body interaction was computed.

Thus it only makes sense to use body particles and develop such a pair style, when particle/particle interactions are more complex than what the *fix rigid* command can already calculate. For example, consider particles with one or more of the following attributes:

- represented by a surface mesh

- represented by a collection of geometric entities (e.g. planes + spheres)
- deformable
- internal stress that induces fragmentation

For these models, the interaction between pairs of particles is likely to be more complex than the summation of simple pairwise interactions. An example is contact or frictional forces between particles with planar surfaces that interpenetrate. Likewise, the body particle may store internal state, such as a stress tensor used to compute a fracture criterion.

These are additional LAMMPS commands that can be used with body particles of different styles

fix nve/body	integrate motion of a body particle in NVE ensemble
fix nvt/body	ditto for NVT ensemble
fix npt/body	ditto for NPT ensemble
fix nph/body	ditto for NPH ensemble
compute body/local	store sub-particle attributes of a body particle
compute temp/body	compute temperature of body particles
dump local	output sub-particle attributes of a body particle
dump image	output body particle attributes as an image

The pair styles defined for use with specific body styles are listed in the sections below.

Specifics of body style nparticle:

The *nparticle* body style represents body particles as a rigid body with a variable number N of sub-particles. It is provided as a vanilla, prototypical example of a body particle, although as mentioned above, the *fix rigid* command already duplicates its functionality.

The atom_style body command for this body style takes two additional arguments:

```
atom_style body nparticle Nmin Nmax
Nmin = minimum # of sub-particles in any body in the system
Nmax = maximum # of sub-particles in any body in the system
```

The Nmin and Nmax arguments are used to bound the size of data structures used internally by each particle.

When the *read_data* command reads a data file for this body style, the following information must be provided for each entry in the *Bodies* section of the data file:

```
atom-ID 1 M
N
ixx iyy izz ixy ixz iyz
x1 y1 z1
...
xN yN zN
```

where M = 6 + 3*N, and N is the number of sub-particles in the body particle.

The integer line has a single value N. The floating point line(s) list 6 moments of inertia followed by the coordinates of the N sub-particles (x1 to zN) as 3N values. These values can be listed on as many lines as you wish; see the *read_data* command for more details.

The 6 moments of inertia (ixx,iyy,izz,ixy,ixz,iyz) should be the values consistent with the current orientation of the rigid body around its center of mass. The values are with respect to the simulation box XYZ axes, not with respect to the principal axes of the rigid body itself. LAMMPS performs the latter calculation internally. The coordinates of each sub-particle are specified as its x,y,z displacement from the center-of-mass of the body particle. The center-of-mass

position of the particle is specified by the x,y,z values in the *Atoms* section of the data file, as is the total mass of the body particle.

The *pair_style body/nparticle* command can be used with this body style to compute body/body and body/non-body interactions.

For output purposes via the *compute body/local* and *dump local* commands, this body style produces one datum for each of the N sub-particles in a body particle. The datum has 3 values:

```
1 = x position of sub-particle
2 = y position of sub-particle
3 = z position of sub-particle
```

These values are the current position of the sub-particle within the simulation domain, not a displacement from the center-of-mass (COM) of the body particle itself. These values are calculated using the current COM and orientation of the body particle.

For images created by the *dump image* command, if the *body* keyword is set, then each body particle is drawn as a collection of spheres, one for each sub-particle. The size of each sphere is determined by the *bflag1* parameter for the *body* keyword. The *bflag2* argument is ignored.

Specifics of body style rounded/polygon:

The *rounded/polygon* body style represents body particles as a 2d polygon with a variable number of N vertices. This style can only be used for 2d models; see the *boundary* command. See the "pair_style body/rounded/polygon" doc page for a diagram of two squares with rounded circles at the vertices. Special cases for N = 1 (circle) and N = 2 (rod with rounded ends) can also be specified.

One use of this body style is for 2d discrete element models, as described in *Fraige*.

Similar to body style *nparticle*, the atom_style body command for this body style takes two additional arguments:

```
atom_style body rounded/polygon Nmin Nmax
Nmin = minimum # of vertices in any body in the system
Nmax = maximum # of vertices in any body in the system
```

The Nmin and Nmax arguments are used to bound the size of data structures used internally by each particle.

When the *read_data* command reads a data file for this body style, the following information must be provided for each entry in the *Bodies* section of the data file:

```
atom-ID 1 M
N
ixx iyy izz ixy ixz iyz
x1 y1 z1
...
xN yN zN
i j j k k ...
diameter
```

where M = 6 + 3*N + 2*N + 1, and N is the number of vertices in the body particle.

The integer line has a single value N. The floating point line(s) list 6 moments of inertia followed by the coordinates of the N vertices (x1 to zN) as 3N values (with z = 0.0 for each), followed by 2N vertex indices corresponding to the end points of the N edges, followed by a single diameter value = the rounded diameter of the circle that surrounds each vertex. The diameter value can be different for each body particle. These floating-point values can be listed on as many lines as you wish; see the *read_data* command for more details.

The 6 moments of inertia (ixx,iyy,izz,ixy,ixz,iyz) should be the values consistent with the current orientation of the rigid body around its center of mass. The values are with respect to the simulation box XYZ axes, not with respect to the principal axes of the rigid body itself. LAMMPS performs the latter calculation internally. The coordinates of each vertex are specified as its x,y,z displacement from the center-of-mass of the body particle. The center-of-mass position of the particle is specified by the x,y,z values in the *Atoms* section of the data file.

For example, the following information would specify a square particle whose edge length is sqrt(2) and rounded diameter is 1.0. The orientation of the square is aligned with the xy coordinate axes which is consistent with the 6 moments of inertia: ixx iyy izz ixy ixz iyz = 1 1 4 0 0 0. Note that only Izz matters in 2D simulations.

```
3 1 27
4
1 1 4 0 0 0
-0.7071 -0.7071 0
-0.7071 0.7071 0
0.7071 0.7071 0
0.7071 -0.7071 0
0 1
1 2
2 3
3 0
1.0
```

A rod in 2D, whose length is 4.0, mass 1.0, rounded at two ends by circles of diameter 0.5, is specified as follows:

```
1 1 13
2
1 1 1.33333 0 0 0
-2 0 0
2 0 0
0.5
```

A disk, whose diameter is 3.0, mass 1.0, is specified as follows:

```
1 1 10
1
1 1 4.5 0 0 0
0 0 0
3.0
```

The *pair_style body/rounded/polygon* command can be used with this body style to compute body/body interactions. The *fix wall/body/polygon* command can be used with this body style to compute the interaction of body particles with a wall.

Specifics of body style rounded/polyhedron:

The *rounded/polyhedron* body style represents body particles as a 3d polyhedron with a variable number of N vertices, E edges and F faces. This style can only be used for 3d models; see the *boundary* command. See the "pair_style body/rounded/polygon" doc page for a diagram of a two 2d squares with rounded circles at the vertices. A 3d cube with rounded spheres at the 8 vertices and 12 rounded edges would be similar. Special cases for N = 1 (sphere) and N = 2 (rod with rounded ends) can also be specified.

This body style is for 3d discrete element models, as described in *Wang*.

Similar to body style *rounded/polygon*, the atom_style body command for this body style takes two additional arguments:

```
atom_style body rounded/polyhedron Nmin Nmax
Nmin = minimum # of vertices in any body in the system
Nmax = maximum # of vertices in any body in the system
```

The Nmin and Nmax arguments are used to bound the size of data structures used internally by each particle.

When the *read_data* command reads a data file for this body style, the following information must be provided for each entry in the *Bodies* section of the data file:

```
atom-ID 3 M
N E F
ixx iyy izz ixy ixz iyz
x1 y1 z1
...
xN yN zN
0 1
1 2
2 3
...
0 1 2 -1
0 2 3 -1
...
1 2 3 4
diameter
```

where M = 6 + 3*N + 2*E + 4*F + 1, and N is the number of vertices in the body particle, E = number of edges, F = number of faces.

The integer line has three values: number of vertices (N), number of edges (E) and number of faces (F). The floating point line(s) list 6 moments of inertia followed by the coordinates of the N vertices (x1 to zN) as 3N values, followed by 2N vertex indices corresponding to the end points of the E edges, then 4*F vertex indices defining F faces. The last value is the diameter value = the rounded diameter of the sphere that surrounds each vertex. The diameter value can be different for each body particle. These floating-point values can be listed on as many lines as you wish; see the *read_data* command for more details. Because the maximum number of vertices per face is hard-coded to be 4 (i.e. quadrilaterals), faces with more than 4 vertices need to be split into triangles or quadrilaterals. For triangular faces, the last vertex index should be set to -1.

The ordering of the 4 vertices within a face should follow the right-hand rule so that the normal vector of the face points outwards from the center of mass.

The 6 moments of inertia (ixx,iyy,izz,ixy,ixz,iyz) should be the values consistent with the current orientation of the rigid body around its center of mass. The values are with respect to the simulation box XYZ axes, not with respect to the principal axes of the rigid body itself. LAMMPS performs the latter calculation internally. The coordinates of each vertex are specified as its x,y,z displacement from the center-of-mass of the body particle. The center-of-mass position of the particle is specified by the x,y,z values in the *Atoms* section of the data file.

For example, the following information would specify a cubic particle whose edge length is 2.0 and rounded diameter is 0.5. The orientation of the cube is aligned with the xyz coordinate axes which is consistent with the 6 moments of inertia: ixx iyy izz ixy ixz iyz = 0.667 0.667 0.667 0 0 0.

```
1 3 79
8 12 6
0.667 0.667 0.667 0 0 0
1 1 1
1 -1 1
-1 -1 1
-1 1 1
1 1 -1
```

(continues on next page)

(continued from previous page)

```
1 -1 -1
-1 -1 -1
-1 1 -1
0 1
1 2
2 3
3 0
4 5
5 6
6 7
7 4
0 4
1 5
2 6
3 7
0 1 2 3
4 5 6 7
0 1 5 4
1 2 6 5
2 3 7 6
3 0 4 7
0.5
```

A rod in 3D, whose length is 4.0, mass 1.0 and rounded at two ends by circles of diameter 0.5, is specified as follows:

```
1 1 13
2
0 1.33333 1.33333 0 0 0
-2 0 0
2 0 0
0.5
```

A sphere whose diameter is 3.0 and mass 1.0, is specified as follows:

```
1 1 10
1
0.9 0.9 0.9 0 0 0
0 0 0
3.0
```

The *pair_style body/rounded/polhedron* command can be used with this body style to compute body/body interactions. The *fix wall/body/polyhedron* command can be used with this body style to compute the interaction of body particles with a wall.

For output purposes via the *compute body/local* and *dump local* commands, this body style produces one datum for each of the N sub-particles in a body particle. The datum has 3 values:

```
1 = x position of vertex
2 = y position of vertex
3 = z position of vertex
```

These values are the current position of the vertex within the simulation domain, not a displacement from the center-of-mass (COM) of the body particle itself. These values are calculated using the current COM and orientation of the body particle.

For images created by the *dump image* command, if the *body* keyword is set, then each body particle is drawn as a polygon consisting of N line segments. Note that the line segments are drawn between the N vertices, which does not correspond exactly to the physical extent of the body (because the *pair_style rounded/polygon* defines finite-size spheres at those point and the line segments between the spheres are tangent to the spheres). The drawn diameter of each line segment is determined by the *bflag1* parameter for the *body* keyword. The *bflag2* argument is ignored.

(Fraige) F. Y. Fraige, P. A. Langston, A. J. Matchett, J. Dodds, Particuology, 6, 455 (2008).

(Wang) J. Wang, H. S. Yu, P. A. Langston, F. Y. Fraige, Granular Matter, 13, 1 (2011).

8.6.4 Polarizable models

In polarizable force fields the charge distributions in molecules and materials respond to their electrostatic environments. Polarizable systems can be simulated in LAMMPS using three methods:

- the fluctuating charge method, implemented in the *QEQ* package,
- the adiabatic core-shell method, implemented in the *CORESHELL* package,
- the thermalized Drude dipole method, implemented in the *USER-DRUDE* package.

The fluctuating charge method calculates instantaneous charges on interacting atoms based on the electronegativity equalization principle. It is implemented in the *fix qeq* which is available in several variants. It is a relatively efficient technique since no additional particles are introduced. This method allows for charge transfer between molecules or atom groups. However, because the charges are located at the interaction sites, off-plane components of polarization cannot be represented in planar molecules or atom groups.

The two other methods share the same basic idea: polarizable atoms are split into one core atom and one satellite particle (called shell or Drude particle) attached to it by a harmonic spring. Both atoms bear a charge and they represent collectively an induced electric dipole. These techniques are computationally more expensive than the QEq method because of additional particles and bonds. These two charge-on-spring methods differ in certain features, with the core-shell model being normally used for ionic/crystalline materials, whereas the so-called Drude model is normally used for molecular systems and fluid states.

The core-shell model is applicable to crystalline materials where the high symmetry around each site leads to stable trajectories of the core-shell pairs. However, bonded atoms in molecules can be so close that a core would interact too strongly or even capture the Drude particle of a neighbor. The Drude dipole model is relatively more complex in order to remedy this and other issues. Specifically, the Drude model includes specific thermostatting of the core-Drude pairs and short-range damping of the induced dipoles.

The three polarization methods can be implemented through a self-consistent calculation of charges or induced dipoles at each timestep. In the fluctuating charge scheme this is done by the matrix inversion method in *fix qeq/point*, but for core-shell or Drude-dipoles the relaxed-dipoles technique would require an slow iterative procedure. These self-consistent solutions yield accurate trajectories since the additional degrees of freedom representing polarization are massless. An alternative is to attribute a mass to the additional degrees of freedom and perform time integration using an extended Lagrangian technique. For the fluctuating charge scheme this is done by *fix qeq/dynamic*, and for the charge-on-spring models by the methods outlined in the next two sections. The assignment of masses to the additional degrees of freedom can lead to unphysical trajectories if care is not exerted in choosing the parameters of the polarizable models and the simulation conditions.

In the core-shell model the vibration of the shells is kept faster than the ionic vibrations to mimic the fast response of the polarizable electrons. But in molecular systems thermalizing the core-Drude pairs at temperatures comparable to the rest of the simulation leads to several problems (kinetic energy transfer, too short a timestep, etc.) In order to avoid these problems the relative motion of the Drude particles with respect to their cores is kept "cold" so the vibration of the core-Drude pairs is very slow, approaching the self-consistent regime. In both models the temperature is regulated using the velocities of the center of mass of core+shell (or Drude) pairs, but in the Drude model the actual relative core-Drude particle motion is thermostatted separately as well.

8.6.5 Adiabatic core/shell model

The adiabatic core-shell model by *Mitchell and Fincham* is a simple method for adding polarizability to a system. In order to mimic the electron shell of an ion, a satellite particle is attached to it. This way the ions are split into a core and a shell where the latter is meant to react to the electrostatic environment inducing polarizability. See the *Howto polarizable* doc page for a discussion of all the polarizable models available in LAMMPS.

Technically, shells are attached to the cores by a spring force f = k*r where k is a parameterized spring constant and r is the distance between the core and the shell. The charges of the core and the shell add up to the ion charge, thus q(ion) = q(core) + q(shell). This setup introduces the ion polarizability (alpha) given by alpha = q(shell)^2 / k. In a similar fashion the mass of the ion is distributed on the core and the shell with the core having the larger mass.

To run this model in LAMMPS, *atom_style full* can be used since atom charge and bonds are needed. Each kind of core/shell pair requires two atom types and a bond type. The core and shell of a core/shell pair should be bonded to each other with a harmonic bond that provides the spring force. For example, a data file for NaCl, as found in examples/coreshell, has this format:

```
432   atoms  # core and shell atoms
216   bonds  # number of core/shell springs

4     atom types  # 2 cores and 2 shells for Na and Cl
2     bond types

0.0 24.09597 xlo xhi
0.0 24.09597 ylo yhi
0.0 24.09597 zlo zhi

Masses       # core/shell mass ratio = 0.1

1 20.690784  # Na core
2 31.90500   # Cl core
3 2.298976   # Na shell
4 3.54500    # Cl shell

Atoms

1    1    2   1.5005    0.00000000   0.00000000   0.00000000 # core of core/shell␣
↪pair 1
2    1    4  -2.5005    0.00000000   0.00000000   0.00000000 # shell of core/shell␣
↪pair 1
3    2    1   1.5056    4.01599500   4.01599500   4.01599500 # core of core/shell␣
↪pair 2
4    2    3  -0.5056    4.01599500   4.01599500   4.01599500 # shell of core/shell␣
↪pair 2
(...)

Bonds   # Bond topology for spring forces

1     2     1     2   # spring for core/shell pair 1
2     2     3     4   # spring for core/shell pair 2
(...)
```

Non-Coulombic (e.g. Lennard-Jones) pairwise interactions are only defined between the shells. Coulombic interactions are defined between all cores and shells. If desired, additional bonds can be specified between cores.

The *special_bonds* command should be used to turn-off the Coulombic interaction within core/shell pairs, since that interaction is set by the bond spring. This is done using the *special_bonds* command with a 1-2 weight = 0.0, which is the default value. It needs to be considered whether one has to adjust the *special_bonds* weighting according to the

molecular topology since the interactions of the shells are bypassed over an extra bond.

Note that this core/shell implementation does not require all ions to be polarized. One can mix core/shell pairs and ions without a satellite particle if desired.

Since the core/shell model permits distances of r = 0.0 between the core and shell, a pair style with a "cs" suffix needs to be used to implement a valid long-range Coulombic correction. Several such pair styles are provided in the CORESHELL package. See *this doc page* for details. All of the core/shell enabled pair styles require the use of a long-range Coulombic solver, as specified by the *kspace_style* command. Either the PPPM or Ewald solvers can be used.

For the NaCL example problem, these pair style and bond style settings are used:

```
pair_style      born/coul/long/cs 20.0 20.0
pair_coeff      * *      0.0 1.000   0.00  0.00   0.00
pair_coeff      3 3    487.0 0.23768 0.00  1.05   0.50 #Na-Na
pair_coeff      3 4 145134.0 0.23768 0.00  6.99   8.70 #Na-Cl
pair_coeff      4 4 405774.0 0.23768 0.00 72.40 145.40 #Cl-Cl

bond_style      harmonic
bond_coeff      1 63.014 0.0
bond_coeff      2 25.724 0.0
```

When running dynamics with the adiabatic core/shell model, the following issues should be considered. The relative motion of the core and shell particles corresponds to the polarization, hereby an instantaneous relaxation of the shells is approximated and a fast core/shell spring frequency ensures a nearly constant internal kinetic energy during the simulation. Thermostats can alter this polarization behavior, by scaling the internal kinetic energy, meaning the shell will not react freely to its electrostatic environment. Therefore it is typically desirable to decouple the relative motion of the core/shell pair, which is an imaginary degree of freedom, from the real physical system. To do that, the *compute temp/cs* command can be used, in conjunction with any of the thermostat fixes, such as *fix nvt* or *fix langevin*. This compute uses the center-of-mass velocity of the core/shell pairs to calculate a temperature, and insures that velocity is what is rescaled for thermostatting purposes. This compute also works for a system with both core/shell pairs and non-polarized ions (ions without an attached satellite particle). The *compute temp/cs* command requires input of two groups, one for the core atoms, another for the shell atoms. Non-polarized ions which might also be included in the treated system should not be included into either of these groups, they are taken into account by the *group-ID* (2nd argument) of the compute. The groups can be defined using the *group *type** command. Note that to perform thermostatting using this definition of temperature, the *fix modify temp* command should be used to assign the compute to the thermostat fix. Likewise the *thermo_modify temp* command can be used to make this temperature be output for the overall system.

For the NaCl example, this can be done as follows:

```
group cores type 1 2
group shells type 3 4
compute CSequ all temp/cs cores shells
fix thermoberendsen all temp/berendsen 1427 1427 0.4    # thermostat for the true␣
↪physical system
fix thermostatequ all nve                                # integrator as needed for␣
↪the berendsen thermostat
fix_modify thermoberendsen temp CSequ
thermo_modify temp CSequ                                 # output of center-of-mass␣
↪derived temperature
```

The pressure for the core/shell system is computed via the regular LAMMPS convention by *treating the cores and shells as individual particles*. For the thermo output of the pressure as well as for the application of a barostat, it is necessary to use an additional *pressure* compute based on the default *temperature* and specifying it as a second argument in *fix modify* and *thermo_modify* resulting in:

```
(...)
compute CSequ all temp/cs cores shells
compute thermo_press_lmp all pressure thermo_temp       # pressure for individual␣
↪particles
thermo_modify temp CSequ press thermo_press_lmp         # modify thermo to regular␣
↪pressure
fix press_bar all npt temp 300 300 0.04 iso 0 0 0.4
fix_modify press_bar temp CSequ press thermo_press_lmp  # pressure modification for␣
↪correct kinetic scalar
```

If *compute temp/cs* is used, the decoupled relative motion of the core and the shell should in theory be stable. However numerical fluctuation can introduce a small momentum to the system, which is noticeable over long trajectories. Therefore it is recommendable to use the *fix momentum* command in combination with *compute temp/cs* when equilibrating the system to prevent any drift.

When initializing the velocities of a system with core/shell pairs, it is also desirable to not introduce energy into the relative motion of the core/shell particles, but only assign a center-of-mass velocity to the pairs. This can be done by using the *bias* keyword of the *velocity create* command and assigning the *compute temp/cs* command to the *temp* keyword of the *velocity* command, e.g.

```
velocity all create 1427 134 bias yes temp CSequ
velocity all scale 1427 temp CSequ
```

To maintain the correct polarizability of the core/shell pairs, the kinetic energy of the internal motion shall remain nearly constant. Therefore the choice of spring force and mass ratio need to ensure much faster relative motion of the 2 atoms within the core/shell pair than their center-of-mass velocity. This allows the shells to effectively react instantaneously to the electrostatic environment and limits energy transfer to or from the core/shell oscillators. This fast movement also dictates the timestep that can be used.

The primary literature of the adiabatic core/shell model suggests that the fast relative motion of the core/shell pairs only allows negligible energy transfer to the environment. The mentioned energy transfer will typically lead to a small drift in total energy over time. This internal energy can be monitored using the *compute chunk/atom* and *compute temp/chunk* commands. The internal kinetic energies of each core/shell pair can then be summed using the sum() special function of the *variable* command. Or they can be time/averaged and output using the *fix ave/time* command. To use these commands, each core/shell pair must be defined as a "chunk". If each core/shell pair is defined as its own molecule, the molecule ID can be used to define the chunks. If cores are bonded to each other to form larger molecules, the chunks can be identified by the *fix property/atom* via assigning a core/shell ID to each atom using a special field in the data file read by the *read_data* command. This field can then be accessed by the *compute property/atom* command, to use as input to the *compute chunk/atom* command to define the core/shell pairs as chunks.

For example if core/shell pairs are the only molecules:

```
read_data NaCl_CS_x0.1_prop.data
compute prop all property/atom molecule
compute cs_chunk all chunk/atom c_prop
compute cstherm all temp/chunk cs_chunk temp internal com yes cdof 3.0     # note the␣
↪chosen degrees of freedom for the core/shell pairs
fix ave_chunk all ave/time 10 1 10 c_cstherm file chunk.dump mode vector
```

For example if core/shell pairs and other molecules are present:

```
fix csinfo all property/atom i_CSID                        # property/atom command
read_data NaCl_CS_x0.1_prop.data fix csinfo NULL CS-Info  # atom property added in␣
↪the data-file
compute prop all property/atom i_CSID
(...)
```

The additional section in the date file would be formatted like this:

```
CS-Info          # header of additional section

1   1            # column 1 = atom ID, column 2 = core/shell ID
2   1
3   2
4   2
5   3
6   3
7   4
8   4
(...)
```

(Mitchell and Fincham) Mitchell, Fincham, J Phys Condensed Matter, 5, 1031-1038 (1993).

(Fincham) Fincham, Mackrodt and Mitchell, J Phys Condensed Matter, 6, 393-404 (1994).

8.6.6 Drude induced dipoles

The thermalized Drude model represents induced dipoles by a pair of charges (the core atom and the Drude particle) connected by a harmonic spring. See the *Howto polarizable* doc page for a discussion of all the polarizable models available in LAMMPS.

The Drude model has a number of features aimed at its use in molecular systems (*Lamoureux and Roux*):

- Thermostatting of the additional degrees of freedom associated with the induced dipoles at very low temperature, in terms of the reduced coordinates of the Drude particles with respect to their cores. This makes the trajectory close to that of relaxed induced dipoles.
- Consistent definition of 1-2 to 1-4 neighbors. A core-Drude particle pair represents a single (polarizable) atom, so the special screening factors in a covalent structure should be the same for the core and the Drude particle. Drude particles have to inherit the 1-2, 1-3, 1-4 special neighbor relations from their respective cores.
- Stabilization of the interactions between induced dipoles. Drude dipoles on covalently bonded atoms interact too strongly due to the short distances, so an atom may capture the Drude particle of a neighbor, or the induced dipoles within the same molecule may align too much. To avoid this, damping at short range can be done by Thole functions (for which there are physical grounds). This Thole damping is applied to the point charges composing the induced dipole (the charge of the Drude particle and the opposite charge on the core, not to the total charge of the core atom).

A detailed tutorial covering the usage of Drude induced dipoles in LAMMPS is on the *Howto drude2e* doc page.

As with the core-shell model, the cores and Drude particles should appear in the data file as standard atoms. The same holds for the springs between them, which are described by standard harmonic bonds. The nature of the atoms (core, Drude particle or non-polarizable) is specified via the *fix drude* command. The special list of neighbors is automatically refactored to account for the equivalence of core and Drude particles as regards special 1-2 to 1-4 screening. It may be necessary to use the *extra/special/per/atom* keyword of the *read_data* command. If using *fix shake*, make sure no Drude particle is in this fix group.

There are two ways to thermostat the Drude particles at a low temperature: use either *fix langevin/drude* for a Langevin thermostat, or *fix drude/transform/** for a Nose-Hoover thermostat. The former requires use of the command *comm_modify vel yes*. The latter requires two separate integration fixes like *nvt* or *npt*. The correct temperatures of the reduced degrees of freedom can be calculated using the *compute temp/drude*. This requires also to use the command *comm_modify vel yes*.

Short-range damping of the induced dipole interactions can be achieved using Thole functions through the *pair style thole* in *pair_style hybrid/overlay* with a Coulomb pair style. It may be useful to use *coul/long/cs* or similar from the CORESHELL package if the core and Drude particle come too close, which can cause numerical issues.

(Lamoureux and Roux) G. Lamoureux, B. Roux, J. Chem. Phys 119, 3025 (2003)

8.6.7 Tutorial for Thermalized Drude oscillators in LAMMPS

This tutorial explains how to use Drude oscillators in LAMMPS to simulate polarizable systems using the USER-DRUDE package. As an illustration, the input files for a simulation of 250 phenol molecules are documented. First of all, LAMMPS has to be compiled with the USER-DRUDE package activated. Then, the data file and input scripts have to be modified to include the Drude dipoles and how to handle them.

Overview of Drude induced dipoles

Polarizable atoms acquire an induced electric dipole moment under the action of an external electric field, for example the electric field created by the surrounding particles. Drude oscillators represent these dipoles by two fixed charges: the core (DC) and the Drude particle (DP) bound by a harmonic potential. The Drude particle can be thought of as the electron cloud whose center can be displaced from the position of the corresponding nucleus.

The sum of the masses of a core-Drude pair should be the mass of the initial (unsplit) atom, $m_C + m_D = m$. The sum of their charges should be the charge of the initial (unsplit) atom, $q_C + q_D = q$. A harmonic potential between the core and Drude partners should be present, with force constant k_D and an equilibrium distance of zero. The (half-)stiffness of the *harmonic bond* $K_D = k_D/2$ and the Drude charge q_D are related to the atom polarizability α by

$$K_D = \frac{1}{2}\frac{q_D^2}{\alpha}$$

Ideally, the mass of the Drude particle should be small, and the stiffness of the harmonic bond should be large, so that the Drude particle remains close ot the core. The values of Drude mass, Drude charge, and force constant can be chosen following different strategies, as in the following examples of polarizable force fields:

- *Lamoureux and Roux* suggest adopting a global half-stiffness, K_D = 500 kcal/(mol Ang ^{2}) - which corresponds to a force constant k_D = 4184 kJ/(mol Ang ^{2}) - for all types of core-Drude bond, a global mass m_D = 0.4 g/mol (or u) for all types of Drude particles, and to calculate the Drude charges for individual atom types from the atom polarizabilities using equation (1). This choice is followed in the polarizable CHARMM force field.
- Alternately *Schroeder and Steinhauser* suggest adopting a global charge q_D = -1.0e and a global mass m_D = 0.1 g/mol (or u) for all Drude particles, and to calculate the force constant for each type of core-Drude bond from equation (1). The timesteps used by these authors are between 0.5 and 2 fs, with the degrees of freedom of the Drude oscillators kept cold at 1 K.
- In both these force fields hydrogen atoms are treated as non-polarizable.

The motion of of the Drude particles can be calculated by minimizing the energy of the induced dipoles at each timestep, by an iterative, self-consistent procedure. The Drude particles can be massless and therefore do not contribute to the kinetic energy. However, the relaxed method is computational slow. An extended-lagrangian method can be used to calculate the positions of the Drude particles, but this requires them to have mass. It is important in this case to decouple the degrees of freedom associated with the Drude oscillators from those of the normal atoms. Thermalizing the Drude dipoles at temperatures comparable to the rest of the simulation leads to several problems (kinetic energy transfer, very short timestep, etc.), which can be remedied by the "cold Drude" technique (*Lamoureux and Roux*).

Two closely related models are used to represent polarization through "charges on a spring": the core-shell model and the Drude model. Although the basic idea is the same, the core-shell model is normally used for ionic/crystalline materials, whereas the Drude model is normally used for molecular systems and fluid states. In ionic crystals the

symmetry around each ion and the distance between them are such that the core-shell model is sufficiently stable. But to be applicable to molecular/covalent systems the Drude model includes two important features:

1. The possibility to thermostat the additional degrees of freedom associated with the induced dipoles at very low temperature, in terms of the reduced coordinates of the Drude particles with respect to their cores. This makes the trajectory close to that of relaxed induced dipoles.
2. The Drude dipoles on covalently bonded atoms interact too strongly due to the short distances, so an atom may capture the Drude particle (shell) of a neighbor, or the induced dipoles within the same molecule may align too much. To avoid this, damping at short of the interactions between the point charges composing the induced dipole can be done by *Thole* functions.

Preparation of the data file

The data file is similar to a standard LAMMPS data file for *atom_style full*. The DPs and the *harmonic bonds* connecting them to their DC should appear in the data file as normal atoms and bonds.

You can use the *polarizer* tool (Python script distributed with the USER-DRUDE package) to convert a non-polarizable data file (here *data.102494.lmp*) to a polarizable data file (*data-p.lmp*)

```
polarizer -q -f phenol.dff data.102494.lmp data-p.lmp
```

This will automatically insert the new atoms and bonds. The masses and charges of DCs and DPs are computed from *phenol.dff*, as well as the DC-DP bond constants. The file *phenol.dff* contains the polarizabilities of the atom types and the mass of the Drude particles, for instance:

```
# units: kJ/mol, A, deg
# kforce is in the form k/2 r_D^2
# type  m_D/u   q_D/e    k_D   alpha/A3  thole
OH      0.4    -1.0    4184.0   0.63     0.67
CA      0.4    -1.0    4184.0   1.36     2.51
CAI     0.4    -1.0    4184.0   1.09     2.51
```

The hydrogen atoms are absent from this file, so they will be treated as non-polarizable atoms. In the non-polarizable data file *data.102494.lmp*, atom names corresponding to the atom type numbers have to be specified as comments at the end of lines of the *Masses* section. You probably need to edit it to add these names. It should look like

```
Masses

1 12.011 # CAI
2 12.011 # CA
3 15.999 # OH
4 1.008  # HA
5 1.008  # HO
```

Basic input file

The atom style should be set to (or derive from) *full*, so that you can define atomic charges and molecular bonds, angles, dihedrals…

The *polarizer* tool also outputs certain lines related to the input script (the use of these lines will be explained below). In order for LAMMPS to recognize that you are using Drude oscillators, you should use the fix *drude*. The command is

```
fix DRUDE all drude C C C N N D D D
```

The N, C, D following the *drude* keyword have the following meaning: There is one tag for each atom type. This tag is C for DCs, D for DPs and N for non-polarizable atoms. Here the atom types 1 to 3 (C and O atoms) are DC, atom types 4 and 5 (H atoms) are non-polarizable and the atom types 6 to 8 are the newly created DPs.

By recognizing the fix *drude*, LAMMPS will find and store matching DC-DP pairs and will treat DP as equivalent to their DC in the *special bonds* relations. It may be necessary to extend the space for storing such special relations. In this case extra space should be reserved by using the *extra/special/per/atom* keyword of either the *read_data* or *create_box* command. With our phenol, there is 1 more special neighbor for which space is required. Otherwise LAMMPS crashes and gives the required value.

```
read_data data-p.lmp extra/special/per/atom 1
```

Let us assume we want to run a simple NVT simulation at 300 K. Note that Drude oscillators need to be thermalized at a low temperature in order to approximate a self-consistent field (SCF), therefore it is not possible to simulate an NVE ensemble with this package. Since dipoles are approximated by a charged DC-DP pair, the *pair_style* must include Coulomb interactions, for instance *lj/cut/coul/long* with *kspace_style pppm*. For example, with a cutoff of 10. and a precision 1.e-4:

```
pair_style lj/cut/coul/long 10.0
kspace_style pppm 1.0e-4
```

As compared to the non-polarizable input file, *pair_coeff* lines need to be added for the DPs. Since the DPs have no Lennard-Jones interactions, their ϵ is 0. so the only *pair_coeff* line that needs to be added is

```
pair_coeff * 6* 0.0 0.0 # All-DPs
```

Now for the thermalization, the simplest choice is to use the *fix langevin/drude*.

```
fix LANG all langevin/drude 300. 100 12435 1. 20 13977
```

This applies a Langevin thermostat at temperature 300. to the centers of mass of the DC-DP pairs, with relaxation time 100 and with random seed 12345. This fix applies also a Langevin thermostat at temperature 1. to the relative motion of the DPs around their DCs, with relaxation time 20 and random seed 13977. Only the DCs and non-polarizable atoms need to be in this fix's group. LAMMPS will thermostat the DPs together with their DC. For this, ghost atoms need to know their velocities. Thus you need to add the following command:

```
comm_modify vel yes
```

In order to avoid that the center of mass of the whole system drifts due to the random forces of the Langevin thermostat on DCs, you can add the *zero yes* option at the end of the fix line.

If the fix *shake* is used to constrain the C-H bonds, it should be invoked after the fix *langevin/drude* for more accuracy.

```
fix SHAKE ATOMS shake 0.0001 20 0 t 4 5
```

Note: The group of the fix *shake* must not include the DPs. If the group *ATOMS* is defined by non-DPs atom types, you could use

Since the fix *langevin/drude* does not perform time integration (just modification of forces but no position/velocity updates), the fix *nve* should be used in conjunction.

```
fix NVE all nve
```

Finally, do not forget to update the atom type elements if you use them in a *dump_modify* ... *element* ... command, by adding the element type of the DPs. Here for instance

```
dump DUMP all custom 10 dump.lammpstrj id mol type element x y z ix iy iz
dump_modify DUMP element C C O H H D D D
```

The input file should now be ready for use!

You will notice that the global temperature *thermo_temp* computed by LAMMPS is not 300. K as wanted. This is because LAMMPS treats DPs as standard atoms in his default compute. If you want to output the temperatures of the DC-DP pair centers of mass and of the DPs relative to their DCs, you should use the *compute temp_drude*

```
compute TDRUDE all temp/drude
```

And then output the correct temperatures of the Drude oscillators using *thermo_style custom* with respectively *c_TDRUDE[1]* and *c_TDRUDE[2]*. These should be close to 300.0 and 1.0 on average.

```
thermo_style custom step temp c_TDRUDE[1] c_TDRUDE[2]
```

Thole screening

Dipolar interactions represented by point charges on springs may not be stable, for example if the atomic polarizability is too high for instance, a DP can escape from its DC and be captured by another DC, which makes the force and energy diverge and the simulation crash. Even without reaching this extreme case, the correlation between nearby dipoles on the same molecule may be exaggerated. Often, special bond relations prevent bonded neighboring atoms to see the charge of each other's DP, so that the problem does not always appear. It is possible to use screened dipole-dipole interactions by using the **pair_style thole**. This is implemented as a correction to the Coulomb pair_styles, which dampens at short distance the interactions between the charges representing the induced dipoles. It is to be used as *hybrid/overlay* with any standard *coul* pair style. In our example, we would use

```
pair_style hybrid/overlay lj/cut/coul/long 10.0 thole 2.6 10.0
```

This tells LAMMPS that we are using two pair_styles. The first one is as above (*lj/cut/coul/long 10.0*). The second one is a *thole* pair_style with default screening factor 2.6 (*Noskov*) and cutoff 10.0.

Since *hybrid/overlay* does not support mixing rules, the interaction coefficients of all the pairs of atom types with i < j should be explicitly defined. The output of the *polarizer* script can be used to complete the *pair_coeff* section of the input file. In our example, this will look like:

```
pair_coeff    1    1 lj/cut/coul/long    0.0700   3.550
pair_coeff    1    2 lj/cut/coul/long    0.0700   3.550
pair_coeff    1    3 lj/cut/coul/long    0.1091   3.310
pair_coeff    1    4 lj/cut/coul/long    0.0458   2.985
pair_coeff    2    2 lj/cut/coul/long    0.0700   3.550
pair_coeff    2    3 lj/cut/coul/long    0.1091   3.310
pair_coeff    2    4 lj/cut/coul/long    0.0458   2.985
pair_coeff    3    3 lj/cut/coul/long    0.1700   3.070
pair_coeff    3    4 lj/cut/coul/long    0.0714   2.745
pair_coeff    4    4 lj/cut/coul/long    0.0300   2.420
pair_coeff    *    5 lj/cut/coul/long    0.0000   0.000
pair_coeff    *   6* lj/cut/coul/long    0.0000   0.000
pair_coeff    1    1 thole   1.090   2.510
pair_coeff    1    2 thole   1.218   2.510
pair_coeff    1    3 thole   0.829   1.590
pair_coeff    1    6 thole   1.090   2.510
pair_coeff    1    7 thole   1.218   2.510
pair_coeff    1    8 thole   0.829   1.590
pair_coeff    2    2 thole   1.360   2.510
```

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```
pair_coeff    2    3 thole   0.926   1.590
pair_coeff    2    6 thole   1.218   2.510
pair_coeff    2    7 thole   1.360   2.510
pair_coeff    2    8 thole   0.926   1.590
pair_coeff    3    3 thole   0.630   0.670
pair_coeff    3    6 thole   0.829   1.590
pair_coeff    3    7 thole   0.926   1.590
pair_coeff    3    8 thole   0.630   0.670
pair_coeff    6    6 thole   1.090   2.510
pair_coeff    6    7 thole   1.218   2.510
pair_coeff    6    8 thole   0.829   1.590
pair_coeff    7    7 thole   1.360   2.510
pair_coeff    7    8 thole   0.926   1.590
pair_coeff    8    8 thole   0.630   0.670
```

For the *thole* pair style the coefficients are

1. the atom polarizability in units of cubic length
2. the screening factor of the Thole function (optional, default value specified by the pair_style command)
3. the cutoff (optional, default value defined by the pair_style command)

The special neighbors have charge-charge and charge-dipole interactions screened by the *coul* factors of the *special_bonds* command (0.0, 0.0, and 0.5 in the example above). Without using the pair_style *thole*, dipole-dipole interactions are screened by the same factor. By using the pair_style *thole*, dipole-dipole interactions are screened by Thole's function, whatever their special relationship (except within each DC-DP pair of course). Consider for example 1-2 neighbors: using the pair_style *thole*, their dipoles will see each other (despite the *coul* factor being 0.) and the interactions between these dipoles will be damped by Thole's function.

Thermostats and barostats

Using a Nose-Hoover barostat with the *langevin/drude* thermostat is straightforward using fix *nph* instead of *nve*. For example:

```
fix NPH all nph iso 1. 1. 500
```

It is also possible to use a Nose-Hoover instead of a Langevin thermostat. This requires to use **fix drude/transform** just before and after the time integration fixes. The *fix drude/transform/direct* converts the atomic masses, positions, velocities and forces into a reduced representation, where the DCs transform into the centers of mass of the DC-DP pairs and the DPs transform into their relative position with respect to their DC. The *fix drude/transform/inverse* performs the reverse transformation. For a NVT simulation, with the DCs and atoms at 300 K and the DPs at 1 K relative to their DC one would use

```
fix DIRECT all drude/transform/direct
fix NVT1 ATOMS nvt temp 300. 300. 100
fix NVT2 DRUDES nvt temp 1. 1. 20
fix INVERSE all drude/transform/inverse
```

For our phenol example, the groups would be defined as

```
group ATOMS  type 1 2 3 4 5 # DCs and non-polarizable atoms
group CORES  type 1 2 3     # DCs
group DRUDES type 6 7 8     # DPs
```

Note that with the fixes *drude/transform*, it is not required to specify *comm_modify vel yes* because the fixes do it anyway (several times and for the forces also). To avoid the flying ice cube artifact *(Lamoureux)*, where the atoms

progressively freeze and the center of mass of the whole system drifts faster and faster, the *fix momentum* can be used. For instance:

```
fix MOMENTUM all momentum 100 linear 1 1 1
```

It is a bit more tricky to run a NPT simulation with Nose-Hoover barostat and thermostat. First, the volume should be integrated only once. So the fix for DCs and atoms should be *npt* while the fix for DPs should be *nvt* (or vice versa). Second, the *fix npt* computes a global pressure and thus a global temperature whatever the fix group. We do want the pressure to correspond to the whole system, but we want the temperature to correspond to the fix group only. We must then use the *fix_modify* command for this. In the end, the block of instructions for thermostatting and barostatting will look like

```
compute TATOMS ATOMS temp
fix DIRECT all drude/transform/direct
fix NPT ATOMS npt temp 300. 300. 100 iso 1. 1. 500
fix_modify NPT temp TATOMS press thermo_press
fix NVT DRUDES nvt temp 1. 1. 20
fix INVERSE all drude/transform/inverse
```

Rigid bodies

You may want to simulate molecules as rigid bodies (but polarizable). Common cases are water models such as *SWM4-NDP*, which is a kind of polarizable TIP4P water. The rigid bodies and the DPs should be integrated separately, even with the Langevin thermostat. Let us review the different thermostats and ensemble combinations.

NVT ensemble using Langevin thermostat:

```
comm_modify vel yes
fix LANG all langevin/drude 300. 100 12435 1. 20 13977
fix RIGID ATOMS rigid/nve/small molecule
fix NVE DRUDES nve
```

NVT ensemble using Nose-Hoover thermostat:

```
fix DIRECT all drude/transform/direct
fix RIGID ATOMS rigid/nvt/small molecule temp 300. 300. 100
fix NVT DRUDES nvt temp 1. 1. 20
fix INVERSE all drude/transform/inverse
```

NPT ensemble with Langevin thermostat:

```
comm_modify vel yes
fix LANG all langevin/drude 300. 100 12435 1. 20 13977
fix RIGID ATOMS rigid/nph/small molecule iso 1. 1. 500
fix NVE DRUDES nve
```

NPT ensemble using Nose-Hoover thermostat:

```
compute TATOM ATOMS temp
fix DIRECT all drude/transform/direct
fix RIGID ATOMS rigid/npt/small molecule temp 300. 300. 100 iso 1. 1. 500
fix_modify RIGID temp TATOM press thermo_press
fix NVT DRUDES nvt temp 1. 1. 20
fix INVERSE all drude/transform/inverse
```

(Lamoureux) Lamoureux and Roux, J Chem Phys, 119, 3025-3039 (2003)

(Schroeder) Schroeder and Steinhauser, J Chem Phys, 133, 154511 (2010).

(Jiang) Jiang, Hardy, Phillips, MacKerell, Schulten, and Roux, J Phys Chem Lett, 2, 87-92 (2011).

(Thole) Chem Phys, 59, 341 (1981).

(Noskov) Noskov, Lamoureux and Roux, J Phys Chem B, 109, 6705 (2005).

(SWM4-NDP) Lamoureux, Harder, Vorobyov, Roux, MacKerell, Chem Phys Let, 418, 245-249 (2006)

8.6.8 Manifolds (surfaces)

Overview:

This doc page is not about a LAMMPS input script command, but about manifolds, which are generalized surfaces, as defined and used by the USER-MANIFOLD package, to track particle motion on the manifolds. See the src/USER-MANIFOLD/README file for more details about the package and its commands.

Below is a list of currently supported manifolds by the USER-MANIFOLD package, their parameters and a short description of them. The parameters listed here are in the same order as they should be passed to the relevant fixes.

manifold	*parameters*	*equation*	*description*
cylinder	R	x^2 + y^2 - R^2 = 0	Cylinder along z-axis, axis going through (0,0,0)
cylinder_dent	R l a	x^2 + y^2 - r(z)^2 = 0, r(x) = R if | z | > l, r(z) = R - a*(1 + cos(z/l))/2 otherwise	A cylinder with a dent around z = 0
dumbbell	a A B c	-(x^2 + y^2) + (a^2 - z^2/c^2) * (1 + (A*sin(B*z^2))^4) = 0	A dumbbell
ellipsoid	a b c	(x/a)^2 + (y/b)^2 + (z/c)^2 = 0	An ellipsoid
gaussian_bump	A l rc1 rc2	if(x < rc1) -z + A * exp(-x^2 / (2 l^2)); else if(x < rc2) -z + a + b*x + c*x^2 + d*x^3; else z	A Gaussian bump at x = y = 0, smoothly tapered to a flat plane z = 0.
plane	a b c x0 y0 z0	a*(x-x0) + b*(y-y0) + c*(z-z0) = 0	A plane with normal (a,b,c) going through point (x0,y0,z0)
plane_wiggle	a w	z - a*sin(w*x) = 0	A plane with a sinusoidal modulation on z along x.
sphere	R	x^2 + y^2 + z^2 - R^2 = 0	A sphere of radius R
supersphere	R q	| x |^q + | y |^q + | z |^q - R^q = 0	A supersphere of hyperradius R
spine	a, A, B, B2, c	-(x^2 + y^2) + (a^2 - z^2/f(z)^2)*(1 + (A*sin(g(z)*z^2))^4), f(z) = c if z > 0, 1 otherwise; g(z) = B if z > 0, B2 otherwise	An approximation to a dendritic spine
spine_two	a, A, B, B2, c	-(x^2 + y^2) + (a^2 - z^2/f(z)^2)*(1 + (A*sin(g(z)*z^2))^2), f(z) = c if z > 0, 1 otherwise; g(z) = B if z > 0, B2 otherwise	Another approximation to a dendritic spine
thylakoid	wB LB lB	Various, see *(Paquay)*	A model grana thylakoid consisting of two block-like compartments connected by a bridge of width wB, length LB and taper length lB
torus	R r	(R - sqrt(x^2 + y^2))^2 + z^2 - r^2	A torus with large radius R and small radius r, centered on (0,0,0)

(Paquay) Paquay and Kusters, Biophys. J., 110, 6, (2016). preprint available at arXiv:1411.3019.

8.6.9 Magnetic spins

The magnetic spin simulations are enabled by the SPIN package, whose implementation is detailed in *Tranchida*.

The model represents the simulation of atomic magnetic spins coupled to lattice vibrations. The dynamics of those magnetic spins can be used to simulate a broad range a phenomena related to magneto-elasticity, or or to study the influence of defects on the magnetic properties of materials.

The magnetic spins are interacting with each others and with the lattice via pair interactions. Typically, the magnetic exchange interaction can be defined using the *pair/spin/exchange* command. This exchange applies a magnetic torque to a given spin, considering the orientation of its neighboring spins and their relative distances. It also applies a force on the atoms as a function of the spin orientations and their associated inter-atomic distances.

The command *fix precession/spin* allows to apply a constant magnetic torque on all the spins in the system. This torque can be an external magnetic field (Zeeman interaction), or an uniaxial magnetic anisotropy.

A Langevin thermostat can be applied to those magnetic spins using *fix langevin/spin*. Typically, this thermostat can be coupled to another Langevin thermostat applied to the atoms using *fix langevin* in order to simulate thermostatted spin-lattice systems.

The magnetic Gilbert damping can also be applied using *fix langevin/spin*. It allows to either dissipate the thermal energy of the Langevin thermostat, or to perform a relaxation of the magnetic configuration toward an equilibrium state.

The command *fix setforce/spin* allows to set the components of the magnetic precession vectors (while erasing and replacing the previously computed magnetic precession vectors on the atom). This command can be used to freeze the magnetic moment of certain atoms in the simulation by zeroing their precession vector.

The command *fix nve/spin* can be used to perform a symplectic integration of the combined dynamics of spins and atomic motions.

The minimization style *min/spin* can be applied to the spins to perform a minimization of the spin configuration.

All the computed magnetic properties can be output by two main commands. The first one is *compute spin*, that enables to evaluate magnetic averaged quantities, such as the total magnetization of the system along x, y, or z, the spin temperature, or the magnetic energy. The second command is *compute property/atom*. It enables to output all the per atom magnetic quantities. Typically, the orientation of a given magnetic spin, or the magnetic force acting on this spin.

(Tranchida) Tranchida, Plimpton, Thibaudeau and Thompson, Journal of Computational Physics, 372, 406-425, (2018).

CHAPTER

NINE

EXAMPLE SCRIPTS

The LAMMPS distribution includes an examples sub-directory with many sample problems. Many are 2d models that run quickly and are straightforward to visualize, requiring at most a couple of minutes to run on a desktop machine. Each problem has an input script (in.*) and produces a log file (log.*) when it runs. Some use a data file (data.*) of initial coordinates as additional input. A few sample log file run on different machines and different numbers of processors are included in the directories to compare your answers to. E.g. a log file like log.date.crack.foo.P means the "crack" example was run on P processors of machine "foo" on that date (i.e. with that version of LAMMPS).

Many of the input files have commented-out lines for creating dump files and image files.

If you uncomment the *dump* command in the input script, a text dump file will be produced, which can be animated by various visualization programs.

If you uncomment the *dump image* command in the input script, and assuming you have built LAMMPS with a JPG library, JPG snapshot images will be produced when the simulation runs. They can be quickly post-processed into a movie using commands described on the *dump image* doc page.

Animations of many of the examples can be viewed on the Movies section of the LAMMPS web site.

There are two kinds of sub-directories in the examples folder. Lower case named directories contain one or a few simple, quick-to-run problems. Upper case named directories contain up to several complex scripts that illustrate a particular kind of simulation method or model. Some of these run for longer times, e.g. to measure a particular quantity.

Lists of both kinds of directories are given below.

9.1 Lowercase directories

accelerate	run with various acceleration options (OpenMP, GPU, Phi)
airebo	polyethylene with AIREBO potential
atm	Axilrod-Teller-Muto potential example
balance	dynamic load balancing, 2d system
body	body particles, 2d system
cmap	CMAP 5-body contributions to CHARMM force field
colloid	big colloid particles in a small particle solvent, 2d system
comb	models using the COMB potential
controller	use of fix controller as a thermostat
coreshell	core/shell model using CORESHELL package
crack	crack propagation in a 2d solid
deposit	deposit atoms and molecules on a surface

Continued on next page

Table 1 – continued from previous page

dipole	point dipolar particles, 2d system
dreiding	methanol via Dreiding FF
eim	NaCl using the EIM potential
ellipse	ellipsoidal particles in spherical solvent, 2d system
flow	Couette and Poiseuille flow in a 2d channel
friction	frictional contact of spherical asperities between 2d surfaces
gcmc	Grand Canonical Monte Carlo (GCMC) via the fix gcmc command
granregion	use of fix wall/region/gran as boundary on granular particles
hugoniostat	Hugoniostat shock dynamics
hyper	global and local hyperdynamics of diffusion on Pt surface
indent	spherical indenter into a 2d solid
kim	use of potentials from the OpenKIM Repository
latte	examples for using fix latte for DFTB via the LATTE library
meam	MEAM test for SiC and shear (same as shear examples)
melt	rapid melt of 3d LJ system
message	demos for LAMMPS client/server coupling with the MESSAGE package
micelle	self-assembly of small lipid-like molecules into 2d bilayers
min	energy minimization of 2d LJ melt
mscg	parameterize a multi-scale coarse-graining (MSCG) model
msst	MSST shock dynamics
nb3b	use of non-bonded 3-body harmonic pair style
neb	nudged elastic band (NEB) calculation for barrier finding
nemd	non-equilibrium MD of 2d sheared system
obstacle	flow around two voids in a 2d channel
peptide	dynamics of a small solvated peptide chain (5-mer)
peri	Peridynamic model of cylinder impacted by indenter
pour	pouring of granular particles into a 3d box, then chute flow
prd	parallel replica dynamics of vacancy diffusion in bulk Si
python	using embedded Python in a LAMMPS input script
qeq	use of the QEQ package for charge equilibration
rdf-adf	computing radial and angle distribution functions for water
reax	RDX and TATB models using the ReaxFF
rerun	use of rerun and read_dump commands
rigid	rigid bodies modeled as independent or coupled
shear	sideways shear applied to 2d solid, with and without a void
snap	NVE dynamics for BCC tantalum crystal using SNAP potential
srd	stochastic rotation dynamics (SRD) particles as solvent
streitz	use of Streitz/Mintmire potential with charge equilibration
tad	temperature-accelerated dynamics of vacancy diffusion in bulk Si
threebody	regression test input for a variety of manybody potentials
vashishta	use of the Vashishta potential
voronoi	Voronoi tesselation via compute voronoi/atom command

Here is how you can run and visualize one of the sample problems:

```
cd indent
cp ../../src/lmp_linux .            # copy LAMMPS executable to this dir
lmp_linux -in in.indent             # run the problem
```

Running the simulation produces the files *dump.indent* and *log.lammps*. You can visualize the dump file of snapshots with a variety of 3rd-party tools highlighted on the Visualization page of the LAMMPS web site.

If you uncomment the *dump image* line(s) in the input script a series of JPG images will be produced by the run (assuming you built LAMMPS with JPG support; see the *Build_settings* doc page for details). These can be viewed individually or turned into a movie or animated by tools like ImageMagick or QuickTime or various Windows-based tools. See the *dump image* doc page for more details. E.g. this Imagemagick command would create a GIF file suitable for viewing in a browser.

```
% convert -loop 1 *.jpg foo.gif
```

9.2 Uppercase directories

ASPHERE	various aspherical particle models, using ellipsoids, rigid bodies, line/triangle particles, etc
COUPLE	examples of how to use LAMMPS as a library
DIFFUSE	compute diffusion coefficients via several methods
ELASTIC	compute elastic constants at zero temperature
ELASTIC_T	compute elastic constants at finite temperature
HEAT	compute thermal conductivity for LJ and water via fix ehex
KAPPA	compute thermal conductivity via several methods
MC	using LAMMPS in a Monte Carlo mode to relax the energy of a system
SPIN	examples for features of the SPIN package
UNITS	examples that run the same simulation in lj, real, metal units
USER	examples for USER packages and USER-contributed commands
VISCOSITY	compute viscosity via several methods

Nearly all of these directories have README files which give more details on how to understand and use their contents.

The USER directory has a large number of sub-directories which correspond by name to a USER package. They contain scripts that illustrate how to use the command(s) provided in that package. Many of the sub-directories have their own README files which give further instructions. See the *Packages_details* doc page for more info on specific USER packages.

CHAPTER

TEN

AUXILIARY TOOLS

LAMMPS is designed to be a computational kernel for performing molecular dynamics computations. Additional pre- and post-processing steps are often necessary to setup and analyze a simulation. A list of such tools can be found on the LAMMPS webpage at these links:

- Pre/Post processing
- Offsite LAMMPS packages & tools
- Pizza.py toolkit

The last link for Pizza.py is a Python-based tool developed at Sandia which provides tools for doing setup, analysis, plotting, and visualization for LAMMPS simulations.

Additional tools included in the LAMMPS distribution are described on this page.

Note that many users write their own setup or analysis tools or use other existing codes and convert their output to a LAMMPS input format or vice versa. The tools listed here are included in the LAMMPS distribution as examples of auxiliary tools. Some of them are not actively supported by the LAMMPS developers, as they were contributed by LAMMPS users. If you have problems using them, we can direct you to the authors.

The source code for each of these codes is in the tools sub-directory of the LAMMPS distribution. There is a Makefile (which you may need to edit for your platform) which will build several of the tools which reside in that directory. Most of them are larger packages in their own sub-directories with their own Makefiles and/or README files.

10.1 Pre-processing tools

amber2lmp	*ch2lmp*	*chain*	*createatoms*	*drude*	*eam database*
eam generate	*eff*	*ipp*	*micelle2d*	*moltemplate*	*msi2lmp*
polybond					

10.2 Post-processing tools

amber2lmp	*binary2txt*	*ch2lmp*	*colvars*	*eff*	*fep*
lmp2arc	*lmp2cfg*	*matlab*	*phonon*	*pymol_asphere*	*python*
reax	*replica*	*smd*	*spin*	*xmgrace*	

10.3 Miscellaneous tools

doxygen	*emacs*	*i-pi*	*kate*	*singularity*
vim				

10.4 Tool descriptions

10.4.1 amber2lmp tool

The amber2lmp sub-directory contains two Python scripts for converting files back-and-forth between the AMBER MD code and LAMMPS. See the README file in amber2lmp for more information.

These tools were written by Keir Novik while he was at Queen Mary University of London. Keir is no longer there and cannot support these tools which are out-of-date with respect to the current LAMMPS version (and maybe with respect to AMBER as well). Since we don't use these tools at Sandia, you will need to experiment with them and make necessary modifications yourself.

10.4.2 binary2txt tool

The file binary2txt.cpp converts one or more binary LAMMPS dump file into ASCII text files. The syntax for running the tool is

```
binary2txt file1 file2 ...
```

which creates file1.txt, file2.txt, etc. This tool must be compiled on a platform that can read the binary file created by a LAMMPS run, since binary files are not compatible across all platforms.

10.4.3 ch2lmp tool

The ch2lmp sub-directory contains tools for converting files back-and-forth between the CHARMM MD code and LAMMPS.

They are intended to make it easy to use CHARMM as a builder and as a post-processor for LAMMPS. Using charmm2lammps.pl, you can convert a PDB file with associated CHARMM info, including CHARMM force field data, into its LAMMPS equivalent. Support for the CMAP correction of CHARMM22 and later is available as an option. This tool can also add solvent water molecules and Na+ or Cl- ions to the system. Using lammps2pdb.pl you can convert LAMMPS atom dumps into PDB files.

See the README file in the ch2lmp sub-directory for more information.

These tools were created by Pieter in't Veld (pjintve at sandia.gov) and Paul Crozier (pscrozi at sandia.gov) at Sandia.

CMAP support added and tested by Xiaohu Hu (hux2 at ornl.gov) and Robert A. Latour (latourr at clemson.edu), David Hyde-Volpe, and Tigran Abramyan, (Clemson University) and Chris Lorenz (chris.lorenz at kcl.ac.uk), King's College London.

10.4.4 chain tool

The file chain.f creates a LAMMPS data file containing bead-spring polymer chains and/or monomer solvent atoms. It uses a text file containing chain definition parameters as an input. The created chains and solvent atoms can strongly overlap, so LAMMPS needs to run the system initially with a "soft" pair potential to un-overlap it. The syntax for running the tool is

```
chain < def.chain > data.file
```

See the def.chain or def.chain.ab files in the tools directory for examples of definition files. This tool was used to create the system for the *chain benchmark*.

10.4.5 colvars tools

The colvars directory contains a collection of tools for post-processing data produced by the colvars collective variable library. To compile the tools, edit the makefile for your system and run "make".

Please report problems and issues the colvars library and its tools at: https://github.com/colvars/colvars/issues

abf_integrate:

MC-based integration of multidimensional free energy gradient Version 20110511

```
Syntax: ./abf_integrate < filename > [-n < nsteps >] [-t < temp >] [-m [0|1]␣
↪(metadynamics)] [-h < hill_height >] [-f < variable_hill_factor >]
```

The LAMMPS interface to the colvars collective variable library, as well as these tools, were created by Axel Kohlmeyer (akohlmey at gmail.com) at ICTP, Italy.

10.4.6 createatoms tool

The tools/createatoms directory contains a Fortran program called createAtoms.f which can generate a variety of interesting crystal structures and geometries and output the resulting list of atom coordinates in LAMMPS or other formats.

See the included Manual.pdf for details.

The tool is authored by Xiaowang Zhou (Sandia), xzhou at sandia.gov.

10.4.7 doxygen tool

The tools/doxygen directory contains a shell script called doxygen.sh which can generate a call graph and API lists using the Doxygen software.

See the included README file for details.

The tool is authored by Nandor Tamaskovics, numericalfreedom at googlemail.com.

10.4.8 drude tool

The tools/drude directory contains a Python script called polarizer.py which can add Drude oscillators to a LAMMPS data file in the required format.

See the header of the polarizer.py file for details.

The tool is authored by Agilio Padua and Alain Dequidt: agilio.padua at univ-bpclermont.fr, alain.dequidt at univ-bpclermont.fr

---

10.4.9 eam database tool

The tools/eam_database directory contains a Fortran program that will generate EAM alloy setfl potential files for any combination of 16 elements: Cu, Ag, Au, Ni, Pd, Pt, Al, Pb, Fe, Mo, Ta, W, Mg, Co, Ti, Zr. The files can then be used with the *pair_style eam/alloy* command.

The tool is authored by Xiaowang Zhou (Sandia), xzhou at sandia.gov, and is based on his paper:

X. W. Zhou, R. A. Johnson, and H. N. G. Wadley, Phys. Rev. B, 69, 144113 (2004).

10.4.10 eam generate tool

The tools/eam_generate directory contains several one-file C programs that convert an analytic formula into a tabulated *embedded atom method (EAM)* setfl potential file. The potentials they produce are in the potentials directory, and can be used with the *pair_style eam/alloy* command.

The source files and potentials were provided by Gerolf Ziegenhain (gerolf at ziegenhain.com).

10.4.11 eff tool

The tools/eff directory contains various scripts for generating structures and post-processing output for simulations using the electron force field (eFF).

These tools were provided by Andres Jaramillo-Botero at CalTech (ajaramil at wag.caltech.edu).

10.4.12 emacs tool

The tools/emacs directory contains an Emacs Lisp add-on file for GNU Emacs that enables a lammps-mode for editing input scripts when using GNU Emacs, with various highlighting options set up.

These tools were provided by Aidan Thompson at Sandia (athomps at sandia.gov).

10.4.13 fep tool

The tools/fep directory contains Python scripts useful for post-processing results from performing free-energy perturbation simulations using the USER-FEP package.

The scripts were contributed by Agilio Padua (Universite Blaise Pascal Clermont-Ferrand), agilio.padua at univ-bpclermont.fr.

See README file in the tools/fep directory.

10.4.14 i-pi tool

The tools/i-pi directory contains a version of the i-PI package, with all the LAMMPS-unrelated files removed. It is provided so that it can be used with the *fix ipi* command to perform path-integral molecular dynamics (PIMD).

The i-PI package was created and is maintained by Michele Ceriotti, michele.ceriotti at gmail.com, to interface to a variety of molecular dynamics codes.

See the tools/i-pi/manual.pdf file for an overview of i-PI, and the *fix ipi* doc page for further details on running PIMD calculations with LAMMPS.

10.4.15 ipp tool

The tools/ipp directory contains a Perl script ipp which can be used to facilitate the creation of a complicated file (say, a lammps input script or tools/createatoms input file) using a template file.

ipp was created and is maintained by Reese Jones (Sandia), rjones at sandia.gov.

See two examples in the tools/ipp directory. One of them is for the tools/createatoms tool's input file.

10.4.16 kate tool

The file in the tools/kate directory is an add-on to the Kate editor in the KDE suite that allow syntax highlighting of LAMMPS input scripts. See the README.txt file for details.

The file was provided by Alessandro Luigi Sellerio (alessandro.sellerio at ieni.cnr.it).

10.4.17 lmp2arc tool

The lmp2arc sub-directory contains a tool for converting LAMMPS output files to the format for Accelrys' Insight MD code (formerly MSI/Biosym and its Discover MD code). See the README file for more information.

This tool was written by John Carpenter (Cray), Michael Peachey (Cray), and Steve Lustig (Dupont). John is now at the Mayo Clinic (jec at mayo.edu), but still fields questions about the tool.

This tool was updated for the current LAMMPS C++ version by Jeff Greathouse at Sandia (jagreat at sandia.gov).

10.4.18 lmp2cfg tool

The lmp2cfg sub-directory contains a tool for converting LAMMPS output files into a series of *.cfg files which can be read into the AtomEye visualizer. See the README file for more information.

This tool was written by Ara Kooser at Sandia (askoose at sandia.gov).

10.4.19 matlab tool

The matlab sub-directory contains several MATLAB scripts for post-processing LAMMPS output. The scripts include readers for log and dump files, a reader for EAM potential files, and a converter that reads LAMMPS dump files and produces CFG files that can be visualized with the AtomEye visualizer.

See the README.pdf file for more information.

These scripts were written by Arun Subramaniyan at Purdue Univ (asubrama at purdue.edu).

10.4.20 micelle2d tool

The file micelle2d.f creates a LAMMPS data file containing short lipid chains in a monomer solution. It uses a text file containing lipid definition parameters as an input. The created molecules and solvent atoms can strongly overlap, so LAMMPS needs to run the system initially with a "soft" pair potential to un-overlap it. The syntax for running the tool is

```
micelle2d < def.micelle2d > data.file
```

See the def.micelle2d file in the tools directory for an example of a definition file. This tool was used to create the system for the *micelle example*.

10.4.21 moltemplate tool

The moltemplate sub-directory contains instructions for installing moltemplate, a Python-based tool for building molecular systems based on a text-file description, and creating LAMMPS data files that encode their molecular topology as lists of bonds, angles, dihedrals, etc. See the README.txt file for more information.

This tool was written by Andrew Jewett (jewett.aij at gmail.com), who supports it. It has its own WWW page at http://moltemplate.org. The latest sources can be found on its GitHub page

---

10.4.22 msi2lmp tool

The msi2lmp sub-directory contains a tool for creating LAMMPS template input and data files from BIOVIA's Materias Studio files (formerly Accelrys' Insight MD code, formerly MSI/Biosym and its Discover MD code).

This tool was written by John Carpenter (Cray), Michael Peachey (Cray), and Steve Lustig (Dupont). Several people contributed changes to remove bugs and adapt its output to changes in LAMMPS.

This tool has several known limitations and is no longer under active development, so there are no changes except for the occasional bug fix.

See the README file in the tools/msi2lmp folder for more information.

10.4.23 phonon tool

The phonon sub-directory contains a post-processing tool useful for analyzing the output of the *fix phonon* command in the USER-PHONON package.

See the README file for instruction on building the tool and what library it needs. And see the examples/USER/phonon directory for example problems that can be post-processed with this tool.

This tool was written by Ling-Ti Kong at Shanghai Jiao Tong University.

10.4.24 polybond tool

The polybond sub-directory contains a Python-based tool useful for performing "programmable polymer bonding". The Python file lmpsdata.py provides a "Lmpsdata" class with various methods which can be invoked by a user-written Python script to create data files with complex bonding topologies.

See the Manual.pdf for details and example scripts.

This tool was written by Zachary Kraus at Georgia Tech.

10.4.25 pymol_asphere tool

The pymol_asphere sub-directory contains a tool for converting a LAMMPS dump file that contains orientation info for ellipsoidal particles into an input file for the PyMol visualization package or its open source variant.

Specifically, the tool triangulates the ellipsoids so they can be viewed as true ellipsoidal particles within PyMol. See the README and examples directory within pymol_asphere for more information.

This tool was written by Mike Brown at Sandia.

10.4.26 python tool

The python sub-directory contains several Python scripts that perform common LAMMPS post-processing tasks, such as:

- extract thermodynamic info from a log file as columns of numbers
- plot two columns of thermodynamic info from a log file using GnuPlot
- sort the snapshots in a dump file by atom ID
- convert multiple *NEB* dump files into one dump file for viz
- convert dump files into XYZ, CFG, or PDB format for viz by other packages

These are simple scripts built on Pizza.py modules. See the README for more info on Pizza.py and how to use these scripts.

10.4.27 replica tool

The tools/replica directory contains the reorder_remd_traj python script which can be used to reorder the replica trajectories (resulting from the use of the temper command) according to temperature. This will produce discontinuous trajectories with all frames at the same temperature in each trajectory. Additional options can be used to calculate the canonical configurational log-weight for each frame at each temperature using the pymbar package. See the README.md file for further details. Try out the peptide example provided.

This tool was written by (and is maintained by) Tanmoy Sanyal, while at the Shell lab at UC Santa Barbara. (tanmoy dot 7989 at gmail.com)

10.4.28 reax tool

The reax sub-directory contains stand-alone codes that can post-process the output of the *fix reax/c/bonds* command from a LAMMPS simulation using *ReaxFF*. See the README.txt file for more info.

These tools were written by Aidan Thompson at Sandia.

10.4.29 smd tool

The smd sub-directory contains a C++ file dump2vtk_tris.cpp and Makefile which can be compiled and used to convert triangle output files created by the Smooth-Mach Dynamics (USER-SMD) package into a VTK-compatible unstructured grid file. It could then be read in and visualized by VTK.

See the header of dump2vtk.cpp for more details.

This tool was written by the USER-SMD package author, Georg Ganzenmuller at the Fraunhofer-Institute for High-Speed Dynamics, Ernst Mach Institute in Germany (georg.ganzenmueller at emi.fhg.de).

10.4.30 spin tool

The spin sub-directory contains a C file interpolate.c which can be compiled and used to perform a cubic polynomial interpolation of the MEP following a GNEB calculation.

See the README file in tools/spin/interpolate_gneb for more details.

This tool was written by the SPIN package author, Julien Tranchida at Sandia National Labs (jtranch at sandia.gov, and by Aleksei Ivanov, at University of Iceland (ali5 at hi.is).

10.4.31 singularity tool

The singularity sub-directory contains container definitions files that can be used to build container images for building and testing LAMMPS on specific OS variants using the Singularity container software. Contributions for additional variants are welcome.

10.4.32 vim tool

The files in the tools/vim directory are add-ons to the VIM editor that allow easier editing of LAMMPS input scripts. See the README.txt file for details.

These files were provided by Gerolf Ziegenhain (gerolf at ziegenhain.com)

10.4.33 xmgrace tool

The files in the tools/xmgrace directory can be used to plot the thermodynamic data in LAMMPS log files via the xmgrace plotting package. There are several tools in the directory that can be used in post-processing mode. The lammpsplot.cpp file can be compiled and used to create plots from the current state of a running LAMMPS simulation.

See the README file for details.

These files were provided by Vikas Varshney (vv0210 at gmail.com)

CHAPTER

ELEVEN

MODIFY & EXTEND LAMMPS

LAMMPS is designed in a modular fashion so as to be easy to modify and extend with new functionality. In fact, about 95% of its source code is add-on files. These doc pages give basic instructions on how to do this.

If you add a new feature to LAMMPS and think it will be of interest to general users, we encourage you to submit it for inclusion in LAMMPS as a pull request on our GitHub site, after reading the *Modify contribute* doc page.

11.1 Overview

The best way to add a new feature to LAMMPS is to find a similar feature and look at the corresponding source and header files to figure out what it does. You will need some knowledge of C++ to be able to understand the high-level structure of LAMMPS and its class organization, but functions (class methods) that do actual computations are written in vanilla C-style code and operate on simple C-style data structures (vectors and arrays).

Most of the new features described on the *Modify* doc page require you to write a new C++ derived class (except for exceptions described below, where you can make small edits to existing files). Creating a new class requires 2 files, a source code file (*.cpp) and a header file (*.h). The derived class must provide certain methods to work as a new option. Depending on how different your new feature is compared to existing features, you can either derive from the base class itself, or from a derived class that already exists. Enabling LAMMPS to invoke the new class is as simple as putting the two source files in the src directory and re-building LAMMPS.

The advantage of C++ and its object-orientation is that all the code and variables needed to define the new feature are in the 2 files you write, and thus shouldn't make the rest of LAMMPS more complex or cause side-effect bugs.

Here is a concrete example. Suppose you write 2 files pair_foo.cpp and pair_foo.h that define a new class PairFoo that computes pairwise potentials described in the classic 1997 *paper* by Foo, et al. If you wish to invoke those potentials in a LAMMPS input script with a command like

```
pair_style foo 0.1 3.5
```

then your pair_foo.h file should be structured as follows:

```
#ifdef PAIR_CLASS
PairStyle(foo,PairFoo)
#else
...
(class definition for PairFoo)
...
#endif
```

where "foo" is the style keyword in the pair_style command, and PairFoo is the class name defined in your pair_foo.cpp and pair_foo.h files.

When you re-build LAMMPS, your new pairwise potential becomes part of the executable and can be invoked with a pair_style command like the example above. Arguments like 0.1 and 3.5 can be defined and processed by your new class.

As illustrated by this example pair style, many kinds of options are referred to in the LAMMPS documentation as the "style" of a particular command.

The *Modify page* lists all the common styles in LAMMPS, and discusses the header file for the base class that these styles are derived from. Public variables in that file are ones used and set by the derived classes which are also used by the base class. Sometimes they are also used by the rest of LAMMPS. Pure functions, which means functions declared as virtual in the base class header file which are also set to 0, are functions you **must** implement in your new derived class to give it the functionality LAMMPS expects. Virtual functions that are not set to 0 are functions you may override or not. Those are usually defined with an empty function body.

Additionally, new output options can be added directly to the thermo.cpp, dump_custom.cpp, and variable.cpp files. These are also listed on the *Modify page*.

Here are additional guidelines for modifying LAMMPS and adding new functionality:

- Think about whether what you want to do would be better as a pre- or post-processing step. Many computations are more easily and more quickly done that way.
- Do not try to do anything within the timestepping of a run that is not parallel. For example do not accumulate a bunch of data on a single processor and analyze it. You run the risk of seriously degrading the parallel efficiency this way.
- If your new feature reads arguments or writes output, make sure you follow the unit conventions discussed by the *units* command.

(Foo) Foo, Morefoo, and Maxfoo, J of Classic Potentials, 75, 345 (1997).

11.2 Submitting new features for inclusion in LAMMPS

We encourage users to submit new features or modifications for LAMMPS to the core developers so they can be added to the LAMMPS distribution. The preferred way to manage and coordinate this is as of Fall 2016 via the LAMMPS project on GitHub. An alternative is to contact the LAMMPS developers or the indicated developer of a package or feature directly and send in your contribution via e-mail.

For any larger modifications or programming project, you are encouraged to contact the LAMMPS developers ahead of time, in order to discuss implementation strategies and coding guidelines, that will make it easier to integrate your contribution and result in less work for everybody involved. You are also encouraged to search through the list of open issues on GitHub and submit a new issue for a planned feature, so you would not duplicate the work of others (and possibly get scooped by them) or have your work duplicated by others.

How quickly your contribution will be integrated depends largely on how much effort it will cause to integrate and test it, how much it requires changes to the core codebase, and of how much interest it is to the larger LAMMPS community. Please see below for a checklist of typical requirements. Once you have prepared everything, see the *Using GitHub with LAMMPS Howto* doc page for instructions on how to submit your changes or new files through a GitHub pull request. If you prefer to submit patches or full files, you should first make certain, that your code works correctly with the latest patch-level version of LAMMPS and contains all bug fixes from it. Then create a gzipped tar file of all changed or added files or a corresponding patch file using 'diff -u' or 'diff -c' and compress it with gzip. Please only use gzip compression, as this works well on all platforms.

If the new features/files are broadly useful we may add them as core files to LAMMPS or as part of a *standard package*. Else we will add them as a user-contributed file or *user package*. Examples of user packages are in src sub-directories that start with USER. The USER-MISC package is simply a collection of (mostly) unrelated single files, which is

the simplest way to have your contribution quickly added to the LAMMPS distribution. All the standard and user packages are listed and described on the *Packages details* doc page.

Note that by providing us files to release, you are agreeing to make them open-source, i.e. we can release them under the terms of the GPL, used as a license for the rest of LAMMPS. See the Open source page on the LAMMPS website for details.

With user packages and files, all we are really providing (aside from the fame and fortune that accompanies having your name in the source code and on the Authors page of the LAMMPS WWW site), is a means for you to distribute your work to the LAMMPS user community, and a mechanism for others to easily try out your new feature. This may help you find bugs or make contact with new collaborators. Note that you're also implicitly agreeing to support your code which means answer questions, fix bugs, and maintain it if LAMMPS changes in some way that breaks it (an unusual event).

Note: If you prefer to actively develop and support your add-on feature yourself, then you may wish to make it available for download from your own website, as a user package that LAMMPS users can add to their copy of LAMMPS. See the Offsite LAMMPS packages and tools page of the LAMMPS web site for examples of groups that do this. We are happy to advertise your package and web site from that page. Simply email the developers with info about your package and we will post it there.

The previous sections of this doc page describe how to add new "style" files of various kinds to LAMMPS. Packages are simply collections of one or more new class files which are invoked as a new style within a LAMMPS input script. If designed correctly, these additions typically do not require changes to the main core of LAMMPS; they are simply add-on files. If you think your new feature requires non-trivial changes in core LAMMPS files, you should communicate with the developers, since we may or may not want to include those changes for some reason. An example of a trivial change is making a parent-class method "virtual" when you derive a new child class from it.

Here is a checklist of steps you need to follow to submit a single file or user package for our consideration. Following these steps will save both you and us time. Please have a look at the existing files in packages in the src directory for examples. If you are uncertain, please ask.

- All source files you provide must compile with the most current version of LAMMPS with multiple configurations. In particular you need to test compiling LAMMPS from scratch with -DLAMMPS_BIGBIG set in addition to the default -DLAMMPS_SMALLBIG setting. Your code will need to work correctly in serial and in parallel using MPI.
- For consistency with the rest of LAMMPS and especially, if you want your contribution(s) to be added to main LAMMPS code or one of its standard packages, it needs to be written in a style compatible with other LAMMPS source files. This means: 2-character indentation per level, **no tabs**, no lines over 80 characters. I/O is done via the C-style stdio library (mixing of stdio and iostreams is generally discouraged), class header files should not import any system headers outside of <cstdio>, STL containers should be avoided in headers, system header from the C library should use the C++-style names (<cstdlib>, <cstdio>, or <cstring>) instead of the C-style names <stdlib.h>, <stdio.h>, or <string.h>), and forward declarations used where possible or needed to avoid including headers. All added code should be placed into the LAMMPS_NS namespace or a sub-namespace; global or static variables should be avoided, as they conflict with the modular nature of LAMMPS and the C++ class structure. Header files must **not** import namespaces with *using*. This all is so the developers can more easily understand, integrate, and maintain your contribution and reduce conflicts with other parts of LAMMPS. This basically means that the code accesses data structures, performs its operations, and is formatted similar to other LAMMPS source files, including the use of the error class for error and warning messages.
- If you want your contribution to be added as a user-contributed feature, and it's a single file (actually a *.cpp and *.h file) it can rapidly be added to the USER-MISC directory. Send us the one-line entry to add to the USER-MISC/README file in that dir, along with the 2 source files. You can do this multiple times if you wish to contribute several individual features.
- If you want your contribution to be added as a user-contribution and it is several related features, it is probably

best to make it a user package directory with a name like USER-FOO. In addition to your new files, the directory should contain a README text file. The README should contain your name and contact information and a brief description of what your new package does. If your files depend on other LAMMPS style files also being installed (e.g. because your file is a derived class from the other LAMMPS class), then an Install.sh file is also needed to check for those dependencies. See other README and Install.sh files in other USER directories as examples. Send us a tarball of this USER-FOO directory.

- Your new source files need to have the LAMMPS copyright, GPL notice, and your name and email address at the top, like other user-contributed LAMMPS source files. They need to create a class that is inside the LAMMPS namespace. If the file is for one of the
- USER packages, including USER-MISC, then we are not as picky about the coding style (see above). I.e. the files do not need to be in the same stylistic format and syntax as other LAMMPS files, though that would be nice for developers as well as users who try to read your code.
- You **must** also create a **documentation** file for each new command or style you are adding to LAMMPS. For simplicity and convenience, the documentation of groups of closely related commands or styles may be combined into a single file. This will be one file for a single-file feature. For a package, it might be several files. These are text files with a .rst extension using the reStructuredText markup language, that are then converted to HTML and PDF using the Sphinx documentation generator tool. Running Sphinx with the included configuration requires Python 3.x. Configuration settings and custom extensions for this conversion are included in the source distribution, and missing python packages will be transparently downloaded into a virtual environment via pip. Thus, if your local system is missing required packages, you need access to the internet. The translation can be as simple as doing "make html pdf" in the doc folder. As appropriate, the text files can include inline mathematical expression or figures (see doc/JPG for examples). Additional PDF files with further details (see doc/PDF for examples) may also be included. The doc page should also include literature citations as appropriate; see the bottom of doc/fix_nh.rst for examples and the earlier part of the same file for how to format the cite itself. Citation labels must be unique across all .rst files. The "Restrictions" section of the doc page should indicate if your command is only available if LAMMPS is built with the appropriate USER-MISC or USER-FOO package. See other user package doc files for examples of how to do this. Please run at least "make html" and "make spelling" and carefully inspect and proofread the resulting HTML format doc page before submitting your code. Upon submission of a pull request, checks for error free completion of the HTML and PDF build will be performed and also a spell check, a check for correct anchors and labels, and a check for completeness of references all styles in their corresponding tables and lists is run. In case the spell check reports false positives they can be added to the file doc/utils/sphinx-config/false_positives.txt
- For a new package (or even a single command) you should include one or more example scripts demonstrating its use. These should run in no more than a couple minutes, even on a single processor, and not require large data files as input. See directories under examples/USER for examples of input scripts other users provided for their packages. These example inputs are also required for validating memory accesses and testing for memory leaks with valgrind
- If there is a paper of yours describing your feature (either the algorithm/science behind the feature itself, or its initial usage, or its implementation in LAMMPS), you can add the citation to the *.cpp source file. See src/USER-EFF/atom_vec_electron.cpp for an example. A LaTeX citation is stored in a variable at the top of the file and a single line of code that references the variable is added to the constructor of the class. Whenever a user invokes your feature from their input script, this will cause LAMMPS to output the citation to a log.cite file and prompt the user to examine the file. Note that you should only use this for a paper you or your group authored. E.g. adding a cite in the code for a paper by Nose and Hoover if you write a fix that implements their integrator is not the intended usage. That kind of citation should just be in the doc page you provide.

Finally, as a general rule-of-thumb, the more clear and self-explanatory you make your documentation and README files, and the easier you make it for people to get started, e.g. by providing example scripts, the more likely it is that users will try out your new feature.

11.3 Atom styles

Classes that define an *atom style* are derived from the AtomVec class and managed by the Atom class. The atom style determines what attributes are associated with an atom. A new atom style can be created if one of the existing atom styles does not define all the attributes you need to store and communicate with atoms.

Atom_vec_atomic.cpp is a simple example of an atom style.

Here is a brief description of methods you define in your new derived class. See atom_vec.h for details.

init	one time setup (optional)
grow	re-allocate atom arrays to longer lengths (required)
grow_reset	make array pointers in Atom and AtomVec classes consistent (required)
copy	copy info for one atom to another atom's array locations (required)
pack_comm	store an atom's info in a buffer communicated every timestep (required)
pack_comm_vel	add velocity info to communication buffer (required)
pack_comm_hybrid	store extra info unique to this atom style (optional)
unpack_comm	retrieve an atom's info from the buffer (required)
unpack_comm_vel	also retrieve velocity info (required)
unpack_comm_hybrid	retrieve extra info unique to this atom style (optional)
pack_reverse	store an atom's info in a buffer communicating partial forces (required)
pack_reverse_hybrid	store extra info unique to this atom style (optional)
unpack_reverse	retrieve an atom's info from the buffer (required)
unpack_reverse_hybrid	retrieve extra info unique to this atom style (optional)
pack_border	store an atom's info in a buffer communicated on neighbor re-builds (required)
pack_border_vel	add velocity info to buffer (required)
pack_border_hybrid	store extra info unique to this atom style (optional)
unpack_border	retrieve an atom's info from the buffer (required)
unpack_border_vel	also retrieve velocity info (required)
unpack_border_hybrid	retrieve extra info unique to this atom style (optional)
pack_exchange	store all an atom's info to migrate to another processor (required)
unpack_exchange	retrieve an atom's info from the buffer (required)
size_restart	number of restart quantities associated with proc's atoms (required)
pack_restart	pack atom quantities into a buffer (required)
unpack_restart	unpack atom quantities from a buffer (required)
create_atom	create an individual atom of this style (required)
data_atom	parse an atom line from the data file (required)
data_atom_hybrid	parse additional atom info unique to this atom style (optional)
data_vel	parse one line of velocity information from data file (optional)
data_vel_hybrid	parse additional velocity data unique to this atom style (optional)
memory_usage	tally memory allocated by atom arrays (required)

The constructor of the derived class sets values for several variables that you must set when defining a new atom style, which are documented in atom_vec.h. New atom arrays are defined in atom.cpp. Search for the word "customize" and you will find locations you will need to modify.

Note: It is possible to add some attributes, such as a molecule ID, to atom styles that do not have them via the *fix property/atom* command. This command also allows new custom attributes consisting of extra integer or floating-point values to be added to atoms. See the *fix property/atom* doc page for examples of cases where this is useful and details on how to initialize, access, and output the custom values.

New *pair styles*, *fixes*, or *computes* can be added to LAMMPS, as discussed below. The code for these classes can use

the per-atom properties defined by fix property/atom. The Atom class has a find_custom() method that is useful in this context:

```
int index = atom->find_custom(char *name, int &flag);
```

The "name" of a custom attribute, as specified in the *fix property/atom* command, is checked to verify that it exists and its index is returned. The method also sets flag = 0/1 depending on whether it is an integer or floating-point attribute. The vector of values associated with the attribute can then be accessed using the returned index as

```
int *ivector = atom->ivector[index];
double *dvector = atom->dvector[index];
```

Ivector or dvector are vectors of length Nlocal = # of owned atoms, which store the attributes of individual atoms.

11.4 Pair styles

Classes that compute pairwise interactions are derived from the Pair class. In LAMMPS, pairwise calculation include many-body potentials such as EAM or Tersoff where particles interact without a static bond topology. New styles can be created to add new pair potentials to LAMMPS.

Pair_lj_cut.cpp is a simple example of a Pair class, though it includes some optional methods to enable its use with rRESPA.

Here is a brief description of the class methods in pair.h:

compute	workhorse routine that computes pairwise interactions
settings	reads the input script line with arguments you define
coeff	set coefficients for one i,j type pair
init_one	perform initialization for one i,j type pair
init_style	initialization specific to this pair style
write & read_restart	write/read i,j pair coeffs to restart files
write & read_restart_settings	write/read global settings to restart files
single	force and energy of a single pairwise interaction between 2 atoms
compute_inner/middle/outer	versions of compute used by rRESPA

The inner/middle/outer routines are optional.

11.5 Bond, angle, dihedral, improper styles

Classes that compute molecular interactions are derived from the Bond, Angle, Dihedral, and Improper classes. New styles can be created to add new potentials to LAMMPS.

Bond_harmonic.cpp is the simplest example of a bond style. Ditto for the harmonic forms of the angle, dihedral, and improper style commands.

Here is a brief description of common methods you define in your new derived class. See bond.h, angle.h, dihedral.h, and improper.h for details and specific additional methods.

init	check if all coefficients are set, calls *init_style* (optional)
init_style	check if style specific conditions are met (optional)
compute	compute the molecular interactions (required)
settings	apply global settings for all types (optional)
coeff	set coefficients for one type (required)
equilibrium_distance	length of bond, used by SHAKE (required, bond only)
equilibrium_angle	opening of angle, used by SHAKE (required, angle only)
write & read_restart	writes/reads coeffs to restart files (required)
single	force and energy of a single bond or angle (required, bond or angle only)
memory_usage	tally memory allocated by the style (optional)

11.6 Compute styles

Classes that compute scalar and vector quantities like temperature and the pressure tensor, as well as classes that compute per-atom quantities like kinetic energy and the centro-symmetry parameter are derived from the Compute class. New styles can be created to add new calculations to LAMMPS.

Compute_temp.cpp is a simple example of computing a scalar temperature. Compute_ke_atom.cpp is a simple example of computing per-atom kinetic energy.

Here is a brief description of methods you define in your new derived class. See compute.h for details.

init	perform one time setup (required)
init_list	neighbor list setup, if needed (optional)
compute_scalar	compute a scalar quantity (optional)
compute_vector	compute a vector of quantities (optional)
compute_peratom	compute one or more quantities per atom (optional)
compute_local	compute one or more quantities per processor (optional)
pack_comm	pack a buffer with items to communicate (optional)
unpack_comm	unpack the buffer (optional)
pack_reverse	pack a buffer with items to reverse communicate (optional)
unpack_reverse	unpack the buffer (optional)
remove_bias	remove velocity bias from one atom (optional)
remove_bias_all	remove velocity bias from all atoms in group (optional)
restore_bias	restore velocity bias for one atom after remove_bias (optional)
restore_bias_all	same as before, but for all atoms in group (optional)
pair_tally_callback	callback function for *tally*-style computes (optional).
memory_usage	tally memory usage (optional)

Tally-style computes are a special case, as their computation is done in two stages: the callback function is registered with the pair style and then called from the Pair::ev_tally() function, which is called for each pair after force and energy has been computed for this pair. Then the tallied values are retrieved with the standard compute_scalar or compute_vector or compute_peratom methods. The USER-TALLY package provides *examples*_compute_tally.html for utilizing this mechanism.

11.7 Fix styles

In LAMMPS, a "fix" is any operation that is computed during timestepping that alters some property of the system. Essentially everything that happens during a simulation besides force computation, neighbor list construction, and output, is a "fix". This includes time integration (update of coordinates and velocities), force constraints or boundary conditions (SHAKE or walls), and diagnostics (compute a diffusion coefficient). New styles can be created to add new options to LAMMPS.

Fix_setforce.cpp is a simple example of setting forces on atoms to prescribed values. There are dozens of fix options already in LAMMPS; choose one as a template that is similar to what you want to implement.

Here is a brief description of methods you can define in your new derived class. See fix.h for details.

setmask	determines when the fix is called during the timestep (required)
init	initialization before a run (optional)
setup_pre_exchange	called before atom exchange in setup (optional)
setup_pre_force	called before force computation in setup (optional)
setup	called immediately before the 1st timestep and after forces are computed (optional)
min_setup_pre_force	like setup_pre_force, but for minimizations instead of MD runs (optional)
min_setup	like setup, but for minimizations instead of MD runs (optional)
initial_integrate	called at very beginning of each timestep (optional)
pre_exchange	called before atom exchange on re-neighboring steps (optional)
pre_neighbor	called before neighbor list build (optional)
pre_force	called before pair & molecular forces are computed (optional)
post_force	called after pair & molecular forces are computed and communicated (optional)
final_integrate	called at end of each timestep (optional)
end_of_step	called at very end of timestep (optional)
write_restart	dumps fix info to restart file (optional)
restart	uses info from restart file to re-initialize the fix (optional)
grow_arrays	allocate memory for atom-based arrays used by fix (optional)
copy_arrays	copy atom info when an atom migrates to a new processor (optional)
pack_exchange	store atom's data in a buffer (optional)
unpack_exchange	retrieve atom's data from a buffer (optional)
pack_restart	store atom's data for writing to restart file (optional)
unpack_restart	retrieve atom's data from a restart file buffer (optional)
size_restart	size of atom's data (optional)
maxsize_restart	max size of atom's data (optional)
setup_pre_force_respa	same as setup_pre_force, but for rRESPA (optional)
initial_integrate_respa	same as initial_integrate, but for rRESPA (optional)
post_integrate_respa	called after the first half integration step is done in rRESPA (optional)
pre_force_respa	same as pre_force, but for rRESPA (optional)
post_force_respa	same as post_force, but for rRESPA (optional)
final_integrate_respa	same as final_integrate, but for rRESPA (optional)
min_pre_force	called after pair & molecular forces are computed in minimizer (optional)
min_post_force	called after pair & molecular forces are computed and communicated in minimizer (optional)
min_store	store extra data for linesearch based minimization on a LIFO stack (optional)
min_pushstore	push the minimization LIFO stack one element down (optional)
min_popstore	pop the minimization LIFO stack one element up (optional)
min_clearstore	clear minimization LIFO stack (optional)
min_step	reset or move forward on line search minimization (optional)
min_dof	report number of degrees of freedom *added* by this fix in minimization (optional)
max_alpha	report maximum allowed step size during linesearch minimization (optional)

Continued on next page

Table 2 – continued from previous page

pack_comm	pack a buffer to communicate a per-atom quantity (optional)
unpack_comm	unpack a buffer to communicate a per-atom quantity (optional)
pack_reverse_comm	pack a buffer to reverse communicate a per-atom quantity (optional)
unpack_reverse_comm	unpack a buffer to reverse communicate a per-atom quantity (optional)
dof	report number of degrees of freedom *removed* by this fix during MD (optional)
compute_scalar	return a global scalar property that the fix computes (optional)
compute_vector	return a component of a vector property that the fix computes (optional)
compute_array	return a component of an array property that the fix computes (optional)
deform	called when the box size is changed (optional)
reset_target	called when a change of the target temperature is requested during a run (optional)
reset_dt	is called when a change of the time step is requested during a run (optional)
modify_param	called when a fix_modify request is executed (optional)
memory_usage	report memory used by fix (optional)
thermo	compute quantities for thermodynamic output (optional)

Typically, only a small fraction of these methods are defined for a particular fix. Setmask is mandatory, as it determines when the fix will be invoked during the timestep. Fixes that perform time integration (*nve*, *nvt*, *npt*) implement initial_integrate() and final_integrate() to perform velocity Verlet updates. Fixes that constrain forces implement post_force().

Fixes that perform diagnostics typically implement end_of_step(). For an end_of_step fix, one of your fix arguments must be the variable "nevery" which is used to determine when to call the fix and you must set this variable in the constructor of your fix. By convention, this is the first argument the fix defines (after the ID, group-ID, style).

If the fix needs to store information for each atom that persists from timestep to timestep, it can manage that memory and migrate the info with the atoms as they move from processors to processor by implementing the grow_arrays, copy_arrays, pack_exchange, and unpack_exchange methods. Similarly, the pack_restart and unpack_restart methods can be implemented to store information about the fix in restart files. If you wish an integrator or force constraint fix to work with rRESPA (see the *run_style* command), the initial_integrate, post_force_integrate, and final_integrate_respa methods can be implemented. The thermo method enables a fix to contribute values to thermodynamic output, as printed quantities and/or to be summed to the potential energy of the system.

11.8 Input script command style

New commands can be added to LAMMPS input scripts by adding new classes that have a "command" method. For example, the create_atoms, read_data, velocity, and run commands are all implemented in this fashion. When such a command is encountered in the LAMMPS input script, LAMMPS simply creates a class with the corresponding name, invokes the "command" method of the class, and passes it the arguments from the input script. The command method can perform whatever operations it wishes on LAMMPS data structures.

The single method your new class must define is as follows:

command	operations performed by the new command

Of course, the new class can define other methods and variables as needed.

11.9 Dump styles

Classes that dump per-atom info to files are derived from the Dump class. To dump new quantities or in a new format, a new derived dump class can be added, but it is typically simpler to modify the DumpCustom class contained in the dump_custom.cpp file.

Dump_atom.cpp is a simple example of a derived dump class.

Here is a brief description of methods you define in your new derived class. See dump.h for details.

write_header	write the header section of a snapshot of atoms
count	count the number of lines a processor will output
pack	pack a proc's output data into a buffer
write_data	write a proc's data to a file

See the *dump* command and its *custom* style for a list of keywords for atom information that can already be dumped by DumpCustom. It includes options to dump per-atom info from Compute classes, so adding a new derived Compute class is one way to calculate new quantities to dump.

Note that new keywords for atom properties are not typically added to the *dump custom* command. Instead they are added to the *compute property/atom* command.

11.10 Kspace styles

Classes that compute long-range Coulombic interactions via K-space representations (Ewald, PPPM) are derived from the KSpace class. New styles can be created to add new K-space options to LAMMPS.

Ewald.cpp is an example of computing K-space interactions.

Here is a brief description of methods you define in your new derived class. See kspace.h for details.

init	initialize the calculation before a run
setup	computation before the 1st timestep of a run
compute	every-timestep computation
memory_usage	tally of memory usage

11.11 Minimization styles

Classes that perform energy minimization derived from the Min class. New styles can be created to add new minimization algorithms to LAMMPS.

Min_cg.cpp is an example of conjugate gradient minimization.

Here is a brief description of methods you define in your new derived class. See min.h for details.

init	initialize the minimization before a run
run	perform the minimization
memory_usage	tally of memory usage

11.12 Region styles

Classes that define geometric regions are derived from the Region class. Regions are used elsewhere in LAMMPS to group atoms, delete atoms to create a void, insert atoms in a specified region, etc. New styles can be created to add new region shapes to LAMMPS.

Region_sphere.cpp is an example of a spherical region.

Here is a brief description of methods you define in your new derived class. See region.h for details.

inside	determine whether a point is in the region
surface_interior	determine if a point is within a cutoff distance inside of surface
surface_exterior	determine if a point is within a cutoff distance outside of surface
shape_update	change region shape if set by time-dependent variable

11.13 Body styles

Classes that define body particles are derived from the Body class. Body particles can represent complex entities, such as surface meshes of discrete points, collections of sub-particles, deformable objects, etc.

See the *Howto body* doc page for an overview of using body particles and the various body styles LAMMPS supports. New styles can be created to add new kinds of body particles to LAMMPS.

Body_nparticle.cpp is an example of a body particle that is treated as a rigid body containing N sub-particles.

Here is a brief description of methods you define in your new derived class. See body.h for details.

data_body	process a line from the Bodies section of a data file
noutrow	number of sub-particles output is generated for
noutcol	number of values per-sub-particle output is generated for
output	output values for the Mth sub-particle
pack_comm_body	body attributes to communicate every timestep
unpack_comm_body	unpacking of those attributes
pack_border_body	body attributes to communicate when reneighboring is done
unpack_border_body	unpacking of those attributes

11.14 Thermodynamic output options

There is one class that computes and prints thermodynamic information to the screen and log file; see the file thermo.cpp.

There are two styles defined in thermo.cpp: "one" and "multi". There is also a flexible "custom" style which allows the user to explicitly list keywords for quantities to print when thermodynamic info is output. See the *thermo_style* command for a list of defined quantities.

The thermo styles (one, multi, etc) are simply lists of keywords. Adding a new style thus only requires defining a new list of keywords. Search for the word "customize" with references to "thermo style" in thermo.cpp to see the two locations where code will need to be added.

New keywords can also be added to thermo.cpp to compute new quantities for output. Search for the word "customize" with references to "keyword" in thermo.cpp to see the several locations where code will need to be added.

Note that the *thermo_style custom* command already allows for thermo output of quantities calculated by *fixes*, *computes*, and *variables*. Thus, it may be simpler to compute what you wish via one of those constructs, than by adding a new keyword to the thermo command.

11.15 Variable options

There is one class that computes and stores *variable* information in LAMMPS; see the file variable.cpp. The value associated with a variable can be periodically printed to the screen via the *print*, *fix print*, or *thermo_style custom* commands. Variables of style "equal" can compute complex equations that involve the following types of arguments:

```
thermo keywords = ke, vol, atoms, ...
other variables = v_a, v_myvar, ...
math functions = div(x,y), mult(x,y), add(x,y), ...
group functions = mass(group), xcm(group,x), ...
atom values = x[123], y[3], vx[34], ...
compute values = c_mytemp[0], c_thermo_press[3], ...
```

Adding keywords for the *thermo_style custom* command (which can then be accessed by variables) is discussed on the *Modify thermo* doc page.

Adding a new math function of one or two arguments can be done by editing one section of the Variable::evaluate() method. Search for the word "customize" to find the appropriate location.

Adding a new group function can be done by editing one section of the Variable::evaluate() method. Search for the word "customize" to find the appropriate location. You may need to add a new method to the Group class as well (see the group.cpp file).

Accessing a new atom-based vector can be done by editing one section of the Variable::evaluate() method. Search for the word "customize" to find the appropriate location.

Adding new *compute styles* (whose calculated values can then be accessed by variables) is discussed on the *Modify compute* doc page.

CHAPTER

TWELVE

USE PYTHON WITH LAMMPS

These doc pages describe various ways that LAMMPS and Python can be used together.

12.1 Overview of Python and LAMMPS

LAMMPS can work together with Python in three ways. First, Python can wrap LAMMPS through the its *library interface*, so that a Python script can create one or more instances of LAMMPS and launch one or more simulations. In Python lingo, this is called "extending" Python with a LAMMPS module.

Second, a lower-level Python interface can be used indirectly through the provided PyLammps and IPyLammps wrapper classes, written in Python. These wrappers try to simplify the usage of LAMMPS in Python by providing an object-based interface to common LAMMPS functionality. They also reduces the amount of code necessary to parameterize LAMMPS scripts through Python and make variables and computes directly accessible.

Third, LAMMPS can use the Python interpreter, so that a LAMMPS input script or styles can invoke Python code directly, and pass information back-and-forth between the input script and Python functions you write. This Python code can also callback to LAMMPS to query or change its attributes through the LAMMPS Python module mentioned above. In Python lingo, this is "embedding" Python in LAMMPS. When used in this mode, Python can perform script operations that the simple LAMMPS input script syntax can not.

12.2 Run LAMMPS from Python

The LAMMPS distribution includes a python directory with all you need to run LAMMPS from Python. The python/lammps.py file wraps the LAMMPS library interface, with one wrapper function per LAMMPS library function. This file makes it is possible to do the following either from a Python script, or interactively from a Python prompt: create one or more instances of LAMMPS, invoke LAMMPS commands or give it an input script, run LAMMPS incrementally, extract LAMMPS results, an modify internal LAMMPS variables. From a Python script you can do this in serial or parallel. Running Python interactively in parallel does not generally work, unless you have a version of Python that extends Python to enable multiple instances of Python to read what you type.

To do all of this, you must first build LAMMPS as a shared library, then insure that your Python can find the python/lammps.py file and the shared library.

Two advantages of using Python to run LAMMPS are how concise the language is, and that it can be run interactively, enabling rapid development and debugging. If you use it to mostly invoke costly operations within LAMMPS, such as running a simulation for a reasonable number of timesteps, then the overhead cost of invoking LAMMPS through Python will be negligible.

The Python wrapper for LAMMPS uses the "ctypes" package in Python, which auto-generates the interface code needed between Python and a set of C-style library functions. Ctypes is part of standard Python for versions 2.5 and later. You can check which version of Python you have by simply typing "python" at a shell prompt.

12.3 Build LAMMPS as a shared library

12.3.1 Build LAMMPS as a shared library using make

Instructions on how to build LAMMPS as a shared library are given on the *Build_basics* doc page. A shared library is one that is dynamically loadable, which is what Python requires to wrap LAMMPS. On Linux this is a library file that ends in ".so", not ".a".

From the src directory, type

```
make foo mode=shlib
```

where foo is the machine target name, such as mpi or serial. This should create the file liblammps_foo.so in the src directory, as well as a soft link liblammps.so, which is what the Python wrapper will load by default. Note that if you are building multiple machine versions of the shared library, the soft link is always set to the most recently built version.

Note: If you are building LAMMPS with an MPI or FFT library or other auxiliary libraries (used by various packages), then all of these extra libraries must also be shared libraries. If the LAMMPS shared-library build fails with an error complaining about this, see the *Build_basics* doc page.

12.3.2 Build LAMMPS as a shared library using CMake

When using CMake the following two options are necessary to generate the LAMMPS shared library:

```
-D BUILD_LIB=on             # enable building LAMMPS as a library
-D BUILD_SHARED_LIBS=on     # enable building of LAMMPS shared library (both options␣
↪are needed!)
```

What this does is create a liblammps.so which contains the majority of LAMMPS code. The generated lmp binary also dynamically links to this library. This means that either this liblammps.so file has to be in the same directory, a system library path (e.g. /usr/lib64/) or in the LD_LIBRARY_PATH.

If you want to use the shared library with Python the recommended way is to create a virtualenv and use it as CMAKE_INSTALL_PREFIX.

```
# create virtualenv
virtualenv --python=$(which python3) myenv3
source myenv3/bin/activate

# build library
mkdir build
cd build
cmake -D PKG_PYTHON=on -D BUILD_LIB=on -D BUILD_SHARED_LIBS=on -D CMAKE_INSTALL_
↪PREFIX=$VIRTUAL_ENV ../cmake
make -j 4

# install into prefix
make install
```

This will also install the Python module into your virtualenv. Since virtualenv doesn't change your LD_LIBRARY_PATH, you still need to add its lib64 folder to it, which contains the installed liblammps.so.

```
export LD_LIBRARY_PATH=$VIRTUAL_ENV/lib64:$LD_LIBRARY_PATH
```

Starting Python outside (!) of your build directory, but with the virtualenv enabled and with the LD_LIBRARY_PATH set gives you access to LAMMPS via Python.

12.4 Installing LAMMPS in Python

For Python to invoke LAMMPS, there are 2 files it needs to know about:

- python/lammps.py
- liblammps.so or liblammps.dylib

The python source code in lammps.py is the Python wrapper on the LAMMPS library interface. The liblammps.so or liblammps.dylib file is the shared LAMMPS library that Python loads dynamically.

You can achieve that Python can find these files in one of two ways:

- set two environment variables pointing to the location in the source tree
- run "make install-python" or run the python/install.py script explicitly

When calling "make install-python" LAMMPS will try to install the python module and the shared library into the python site-packages folders; either the system-wide ones, or the local users ones (in case of insufficient permissions for the global install). Python will then find the module and shared library file automatically. The exact location of these folders depends on your python version and your operating system. When using the CMake build system, you can set the python executable to use during the CMake configuration process. Details are given in the build instructions for the *PYTHON* package. When using the conventional make system, you can override the python version to version x.y when calling make with PYTHON=pythonx.y.

If you set the paths to these files as environment variables, you only have to do it once. For the csh or tcsh shells, add something like this to your ~/.cshrc file, one line for each of the two files:

```
setenv PYTHONPATH ${PYTHONPATH}:/home/sjplimp/lammps/python
setenv LD_LIBRARY_PATH ${LD_LIBRARY_PATH}:/home/sjplimp/lammps/src
```

On MacOSX you may also need to set DYLD_LIBRARY_PATH accordingly. For Bourne/Korn shells accordingly into the corresponding files using the "export" shell builtin.

If you use "make install-python" or the python/install.py script, you need to invoke it every time you rebuild LAMMPS (as a shared library) or make changes to the python/lammps.py file, so that the site-packages files are updated with the new version.

If the default settings of "make install-python" are not what you want, you can invoke install.py from the python directory manually as

```
% python install.py -m <python module> -l <shared library> -v <version.h file>
↪ [-d <pydir>]
```

- The -m flag points to the lammps.py python module file to be installed,
- the -l flag points to the LAMMPS shared library file to be installed,
- the -v flag points to the version.h file in the LAMMPS source
- and the optional -d flag to a custom (legacy) installation folder

If you use a legacy installation folder, you will need to set your PYTHONPATH and LD_LIBRARY_PATH (and/or DYLD_LIBRARY_PATH) environment variables accordingly, as described above.

Note that if you want Python to be able to load different versions of the LAMMPS shared library (see *this section*), you will need to manually copy files like liblammps_g++.so into the appropriate system directory. This is not needed if you set the LD_LIBRARY_PATH environment variable as described above.

12.5 Extending Python to run in parallel

If you wish to run LAMMPS in parallel from Python, you need to extend your Python with an interface to MPI. This also allows you to make MPI calls directly from Python in your script, if you desire.

We have tested this with mpi4py and pypar:

- MPI for Python
- pypar

We recommend the use of mpi4py as it is the more complete MPI interface, and as of version 2.0.0 mpi4py allows passing a custom MPI communicator to the LAMMPS constructor, which means one can easily run one or more LAMMPS instances on subsets of the total MPI ranks.

To install mpi4py (version mpi4py-3.0.3 as of Nov 2019), unpack it and from its main directory, type

```
python setup.py build
sudo python setup.py install
```

Again, the "sudo" is only needed if required to copy mpi4py files into your Python distribution's site-packages directory. To install with user privilege into the user local directory type

```
python setup.py install --user
```

If you have successfully installed mpi4py, you should be able to run Python and type

```
from mpi4py import MPI
```

without error. You should also be able to run python in parallel on a simple test script

```
% mpirun -np 4 python test.py
```

where test.py contains the lines

```
from mpi4py import MPI
comm = MPI.COMM_WORLD
print "Proc %d out of %d procs" % (comm.Get_rank(),comm.Get_size())
```

and see one line of output for each processor you run on.

Note: To use mpi4py and LAMMPS in parallel from Python, you must insure both are using the same version of MPI. If you only have one MPI installed on your system, this is not an issue, but it can be if you have multiple MPIs. Your LAMMPS build is explicit about which MPI it is using, since you specify the details in your low-level src/MAKE/Makefile.foo file. Mpi4py uses the "mpicc" command to find information about the MPI it uses to build against. And it tries to load "libmpi.so" from the LD_LIBRARY_PATH. This may or may not find the MPI library that LAMMPS is using. If you have problems running both mpi4py and LAMMPS together, this is an issue you may need to address, e.g. by moving other MPI installations so that mpi4py finds the right one.

12.6 Test the Python/LAMMPS interface

To test if LAMMPS is callable from Python, launch Python interactively and type:

```
>>> from lammps import lammps
>>> lmp = lammps()
```

If you get no errors, you're ready to use LAMMPS from Python. If the 2nd command fails, the most common error to see is

```
OSError: Could not load LAMMPS dynamic library
```

which means Python was unable to load the LAMMPS shared library. This typically occurs if the system can't find the LAMMPS shared library or one of the auxiliary shared libraries it depends on, or if something about the library is incompatible with your Python. The error message should give you an indication of what went wrong.

You can also test the load directly in Python as follows, without first importing from the lammps.py file:

```
>>> from ctypes import CDLL
>>> CDLL("liblammps.so")
```

If an error occurs, carefully go through the steps on the *Build_basics* doc page about building a shared library and the *Python_install* doc page about insuring Python can find the necessary two files it needs.

12.6.1 Test LAMMPS and Python in serial:

To run a LAMMPS test in serial, type these lines into Python interactively from the bench directory:

```
>>> from lammps import lammps
>>> lmp = lammps()
>>> lmp.file("in.lj")
```

Or put the same lines in the file test.py and run it as

```
% python test.py
```

Either way, you should see the results of running the in.lj benchmark on a single processor appear on the screen, the same as if you had typed something like:

```
lmp_g++ -in in.lj
```

12.6.2 Test LAMMPS and Python in parallel:

To run LAMMPS in parallel, assuming you have installed the PyPar package as discussed above, create a test.py file containing these lines:

```
import pypar
from lammps import lammps
lmp = lammps()
lmp.file("in.lj")
print "Proc %d out of %d procs has" % (pypar.rank(),pypar.size()),lmp
pypar.finalize()
```

To run LAMMPS in parallel, assuming you have installed the mpi4py package as discussed above, create a test.py file containing these lines:

```
from mpi4py import MPI
from lammps import lammps
lmp = lammps()
lmp.file("in.lj")
me = MPI.COMM_WORLD.Get_rank()
nprocs = MPI.COMM_WORLD.Get_size()
print "Proc %d out of %d procs has" % (me,nprocs),lmp
MPI.Finalize()
```

You can either script in parallel as:

```
% mpirun -np 4 python test.py
```

and you should see the same output as if you had typed

```
% mpirun -np 4 lmp_g++ -in in.lj
```

Note that if you leave out the 3 lines from test.py that specify PyPar commands you will instantiate and run LAMMPS independently on each of the P processors specified in the mpirun command. In this case you should get 4 sets of output, each showing that a LAMMPS run was made on a single processor, instead of one set of output showing that LAMMPS ran on 4 processors. If the 1-processor outputs occur, it means that PyPar is not working correctly.

Also note that once you import the PyPar module, PyPar initializes MPI for you, and you can use MPI calls directly in your Python script, as described in the PyPar documentation. The last line of your Python script should be pypar.finalize(), to insure MPI is shut down correctly.

12.6.3 Running Python scripts:

Note that any Python script (not just for LAMMPS) can be invoked in one of several ways:

```
% python foo.script
% python -i foo.script
% foo.script
```

The last command requires that the first line of the script be something like this:

```
#!/usr/local/bin/python
#!/usr/local/bin/python -i
```

where the path points to where you have Python installed, and that you have made the script file executable:

```
% chmod +x foo.script
```

Without the "-i" flag, Python will exit when the script finishes. With the "-i" flag, you will be left in the Python interpreter when the script finishes, so you can type subsequent commands. As mentioned above, you can only run Python interactively when running Python on a single processor, not in parallel.

12.7 Python library interface

As described previously, the Python interface to LAMMPS consists of a Python "lammps" module, the source code for which is in python/lammps.py, which creates a "lammps" object, with a set of methods that can be invoked on that object. The sample Python code below assumes you have first imported the "lammps" module in your Python script, as follows:

```
from lammps import lammps
```

These are the methods defined by the lammps module. If you look at the files src/library.cpp and src/library.h you will see they correspond one-to-one with calls you can make to the LAMMPS library from a C++ or C or Fortran program, and which are described on the *Howto library* doc page.

The python/examples directory has Python scripts which show how Python can run LAMMPS, grab data, change it, and put it back into LAMMPS.

```
lmp = lammps()            # create a LAMMPS object using the default liblammps.so␣
↪library
                          # 4 optional args are allowed: name, cmdargs, ptr, comm
lmp = lammps(ptr=lmpptr) # use lmpptr as previously created LAMMPS object
lmp = lammps(comm=split) # create a LAMMPS object with a custom communicator,␣
↪requires mpi4py 2.0.0 or later
lmp = lammps(name="g++")    # create a LAMMPS object using the liblammps_g++.so library
lmp = lammps(name="g++",cmdargs=list)     # add LAMMPS command-line args, e.g. list = [
↪"-echo","screen"]

lmp.close()               # destroy a LAMMPS object

version = lmp.version()  # return the numerical version id, e.g. LAMMPS 2 Sep 2015 ->␣
↪20150902

lmp.file(file)            # run an entire input script, file = "in.lj"
lmp.command(cmd)          # invoke a single LAMMPS command, cmd = "run 100"
lmp.commands_list(cmdlist)      # invoke commands in cmdlist = **"run 10", "run 20"**
lmp.commands_string(multicmd)  # invoke commands in multicmd = "run 10\nrun 20"

size = lmp.extract_setting(name)      # return data type info

xlo = lmp.extract_global(name,type)  # extract a global quantity
                                     # name = "boxxlo", "nlocal", etc
                                     # type = 0 = int
                                     #        1 = double

boxlo,boxhi,xy,yz,xz,periodicity,box_change = lmp.extract_box()  # extract box info

coords = lmp.extract_atom(name,type)       # extract a per-atom quantity
                                           # name = "x", "type", etc
                                           # type = 0 = vector of ints
                                           #        1 = array of ints
                                           #        2 = vector of doubles
                                           #        3 = array of doubles

eng = lmp.extract_compute(id,style,type)  # extract value(s) from a compute
v3 = lmp.extract_fix(id,style,type,i,j)   # extract value(s) from a fix
                                           # id = ID of compute or fix
                                           # style = 0 = global data
                                           #         1 = per-atom data
```

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```
                                        #         2 = local data
                                        # type = 0 = scalar
                                        #        1 = vector
                                        #        2 = array
                                        # i,j = indices of value in global vector␣
↪or array

var = lmp.extract_variable(name,group,flag)  # extract value(s) from a variable
                                             # name = name of variable
                                             # group = group ID (ignored for equal-
↪style variables)
                                             # flag = 0 = equal-style variable
                                             #        1 = atom-style variable

value = lmp.get_thermo(name)                # return current value of a thermo keyword
natoms = lmp.get_natoms()                   # total # of atoms as int

flag = lmp.set_variable(name,value)         # set existing named string-style variable␣
↪to value, flag = 0 if successful
lmp.reset_box(boxlo,boxhi,xy,yz,xz)         # reset the simulation box size

data = lmp.gather_atoms(name,type,count)    # return per-atom property of all atoms␣
↪gathered into data, ordered by atom ID
                                            # name = "x", "charge", "type", etc
data = lmp.gather_atoms_concat(name,type,count)  # ditto, but concatenated atom␣
↪values from each proc (unordered)
data = lmp.gather_atoms_subset(name,type,count,ndata,ids)  # ditto, but for subset of␣
↪Ndata atoms with IDs

lmp.scatter_atoms(name,type,count,data)     # scatter per-atom property to all atoms␣
↪from data, ordered by atom ID
                                            # name = "x", "charge", "type", etc
                                            # count = # of per-atom values, 1 or 3, etc

lmp.scatter_atoms_subset(name,type,count,ndata,ids,data)  # ditto, but for subset of␣
↪Ndata atoms with IDs

lmp.create_atoms(n,ids,types,x,v,image,shrinkexceed)   # create N atoms with IDs,␣
↪types, x, v, and image flags
```

The lines

```
from lammps import lammps
lmp = lammps()
```

create an instance of LAMMPS, wrapped in a Python class by the lammps Python module, and return an instance of the Python class as lmp. It is used to make all subsequent calls to the LAMMPS library.

Additional arguments to lammps() can be used to tell Python the name of the shared library to load or to pass arguments to the LAMMPS instance, the same as if LAMMPS were launched from a command-line prompt.

If the ptr argument is set like this:

```
lmp = lammps(ptr=lmpptr)
```

then lmpptr must be an argument passed to Python via the LAMMPS *python* command, when it is used to define a Python function that is invoked by the LAMMPS input script. This mode of calling Python from LAMMPS is

described in the *Python call* doc page. The variable lmpptr refers to the instance of LAMMPS that called the embedded Python interpreter. Using it as an argument to lammps() allows the returned Python class instance "lmp" to make calls to that instance of LAMMPS. See the *python* command doc page for examples using this syntax.

Note that you can create multiple LAMMPS objects in your Python script, and coordinate and run multiple simulations, e.g.

```
from lammps import lammps
lmp1 = lammps()
lmp2 = lammps()
lmp1.file("in.file1")
lmp2.file("in.file2")
```

The file(), command(), commands_list(), commands_string() methods allow an input script, a single command, or multiple commands to be invoked.

The extract_setting(), extract_global(), extract_box(), extract_atom(), extract_compute(), extract_fix(), and extract_variable() methods return values or pointers to data structures internal to LAMMPS.

For extract_global() see the src/library.cpp file for the list of valid names. New names could easily be added. A double or integer is returned. You need to specify the appropriate data type via the type argument.

For extract_atom(), a pointer to internal LAMMPS atom-based data is returned, which you can use via normal Python subscripting. See the extract() method in the src/atom.cpp file for a list of valid names. Again, new names could easily be added if the property you want is not listed. A pointer to a vector of doubles or integers, or a pointer to an array of doubles (double **) or integers (int **) is returned. You need to specify the appropriate data type via the type argument.

For extract_compute() and extract_fix(), the global, per-atom, or local data calculated by the compute or fix can be accessed. What is returned depends on whether the compute or fix calculates a scalar or vector or array. For a scalar, a single double value is returned. If the compute or fix calculates a vector or array, a pointer to the internal LAMMPS data is returned, which you can use via normal Python subscripting. The one exception is that for a fix that calculates a global vector or array, a single double value from the vector or array is returned, indexed by I (vector) or I and J (array). I,J are zero-based indices. The I,J arguments can be left out if not needed. See the *Howto output* doc page for a discussion of global, per-atom, and local data, and of scalar, vector, and array data types. See the doc pages for individual *computes* and *fixes* for a description of what they calculate and store.

For extract_variable(), an *equal-style or atom-style variable* is evaluated and its result returned.

For equal-style variables a single double value is returned and the group argument is ignored. For atom-style variables, a vector of doubles is returned, one value per atom, which you can use via normal Python subscripting. The values will be zero for atoms not in the specified group.

The get_thermo() method returns the current value of a thermo keyword as a float.

The get_natoms() method returns the total number of atoms in the simulation, as an int.

The set_variable() method sets an existing string-style variable to a new string value, so that subsequent LAMMPS commands can access the variable.

The reset_box() method resets the size and shape of the simulation box, e.g. as part of restoring a previously extracted and saved state of a simulation.

The gather methods collect peratom info of the requested type (atom coords, atom types, forces, etc) from all processors, and returns the same vector of values to each calling processor. The scatter functions do the inverse. They distribute a vector of peratom values, passed by all calling processors, to individual atoms, which may be owned by different processors.

Note that the data returned by the gather methods, e.g. gather_atoms("x"), is different from the data structure returned by extract_atom("x") in four ways. (1) Gather_atoms() returns a vector which you index as x[i]; extract_atom() returns an array which you index as x[i][j]. (2) Gather_atoms() orders the atoms by atom ID while extract_atom() does not.

(3) Gather_atoms() returns a list of all atoms in the simulation; extract_atoms() returns just the atoms local to each processor. (4) Finally, the gather_atoms() data structure is a copy of the atom coords stored internally in LAMMPS, whereas extract_atom() returns an array that effectively points directly to the internal data. This means you can change values inside LAMMPS from Python by assigning a new values to the extract_atom() array. To do this with the gather_atoms() vector, you need to change values in the vector, then invoke the scatter_atoms() method.

For the scatter methods, the array of coordinates passed to must be a ctypes vector of ints or doubles, allocated and initialized something like this:

```
from ctypes import \*
natoms = lmp.get_natoms()
n3 = 3\*natoms
x = (n3\*c_double)()
x[0] = x coord of atom with ID 1
x[1] = y coord of atom with ID 1
x[2] = z coord of atom with ID 1
x[3] = x coord of atom with ID 2
...
x[n3-1] = z coord of atom with ID natoms
lmp.scatter_atoms("x",1,3,x)
```

Alternatively, you can just change values in the vector returned by the gather methods, since they are also ctypes vectors.

As noted above, these Python class methods correspond one-to-one with the functions in the LAMMPS library interface in src/library.cpp and library.h. This means you can extend the Python wrapper via the following steps:

- Add a new interface function to src/library.cpp and src/library.h.
- Rebuild LAMMPS as a shared library.
- Add a wrapper method to python/lammps.py for this interface function.
- You should now be able to invoke the new interface function from a Python script.

---

class lammps.**lammps**(*name=''*, *cmdargs=None*, *ptr=None*, *comm=None*)

find_compute_neighlist(*computeid*, *request=0*)

Find neighbor list index of compute neighbor list

Parameters

- **computeid** (*string*) – name of compute
- **request** (*int, optional*) – index of neighbor list request, in case there are more than one, defaults to 0

Returns neighbor list index if found, otherwise -1

Return type int

find_fix_neighlist(*fixid*, *request=0*)

Find neighbor list index of fix neighbor list

Parameters

- **fixid** (*string*) – name of fix
- **request** (*int, optional*) – index of neighbor list request, in case there are more than one, defaults to 0

Returns neighbor list index if found, otherwise -1

Return type int

find_pair_neighlist(*style*, *exact=True*, *nsub=0*, *request=0*)

Find neighbor list index of pair style neighbor list

Try finding pair instance that matches style. If exact is set, the pair must match style exactly. If exact is 0, style must only be contained. If pair is of style pair/hybrid, style is instead matched the nsub-th hybrid sub-style.

Once the pair instance has been identified, multiple neighbor list requests may be found. Every neighbor list is uniquely identified by its request index. Thus, providing this request index ensures that the correct neighbor list index is returned.

Parameters

- **style** (*string*) – name of pair style that should be searched for
- **exact** (*bool, optional*) – controls whether style should match exactly or only must be contained in pair style name, defaults to True
- **nsub** (*int, optional*) – match nsub-th hybrid sub-style, defaults to 0
- **request** (*int, optional*) – index of neighbor list request, in case there are more than one, defaults to 0

Returns neighbor list index if found, otherwise -1

Return type int

get_neighlist(*idx*)

Returns an instance of `NeighList` which wraps access to the neighbor list with the given index

Parameters **idx** (*int*) – index of neighbor list

Returns an instance of `NeighList` wrapping access to neighbor list data

Return type *NeighList*

get_neighlist_element_neighbors(*idx*, *element*)

Return data of neighbor list entry

Parameters

- **element** (*int*) – neighbor list index
- **element** – neighbor list element index

Returns tuple with atom local index, number of neighbors and array of neighbor local atom indices

Return type (int, int, numpy.array)

get_neighlist_size(*idx*)

Return the number of elements in neighbor list with the given index

Parameters **idx** (*int*) – neighbor list index

Returns number of elements in neighbor list with index idx

Return type int

property has_exceptions

Return whether the LAMMPS shared library was compiled with C++ exceptions handling enabled

class lammps.**NeighList**(*lmp*, *idx*)

This is a wrapper class that exposes the contents of a neighbor list

It can be used like a regular Python list.

Internally it uses the lower-level LAMMPS C-library interface.

Parameters

- **lmp** (lammps) – reference to instance of *lammps*
- **idx** (*int*) – neighbor list index

get(*element*)

Returns tuple with atom local index, number of neighbors and array of neighbor local atom indices

Return type (int, int, numpy.array)

property size

Returns number of elements in neighbor list

12.8 PyLammps interface

PyLammps is a Python wrapper class which can be created on its own or use an existing lammps Python object. It has its own *Howto pylammps* doc page.

12.9 Example Python scripts that use LAMMPS

These are the Python scripts included as demos in the python/examples directory of the LAMMPS distribution, to illustrate the kinds of things that are possible when Python wraps LAMMPS. If you create your own scripts, send them to us and we can include them in the LAMMPS distribution.

trivial.py	read/run a LAMMPS input script through Python
demo.py	invoke various LAMMPS library interface routines
simple.py	run in parallel
similar to examples/COUPLE/simple/simple.cpp	split.py
same as simple.py but running in parallel on a subset of procs	gui.py
GUI go/stop/temperature-slider to control LAMMPS	plot.py
real-time temperature plot with GnuPlot via Pizza.py	viz_tool.py
real-time viz via some viz package	vizplotgui_tool.py
combination of viz_tool.py and plot.py and gui.py	

For the viz_tool.py and vizplotgui_tool.py commands, replace "tool" with "gl" or "atomeye" or "pymol" or "vmd", depending on what visualization package you have installed.

Note that for GL, you need to be able to run the Pizza.py GL tool, which is included in the pizza sub-directory. See the Pizza.py doc pages for more info:

Note that for AtomEye, you need version 3, and there is a line in the scripts that specifies the path and name of the executable. See the AtomEye WWW pages here or here for more details:

```
http://mt.seas.upenn.edu/Archive/Graphics/A
http://mt.seas.upenn.edu/Archive/Graphics/A3/A3.html
```

The latter link is to AtomEye 3 which has the scripting capability needed by these Python scripts.

Note that for PyMol, you need to have built and installed the open-source version of PyMol in your Python, so that you can import it from a Python script. See the PyMol WWW pages here or here for more details:

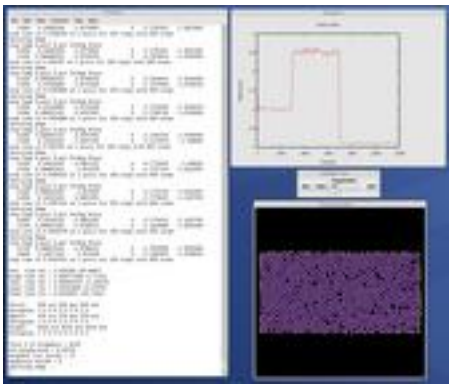
```
http://www.pymol.org
http://sourceforge.net/scm/?type=svn&group_id=4546
```

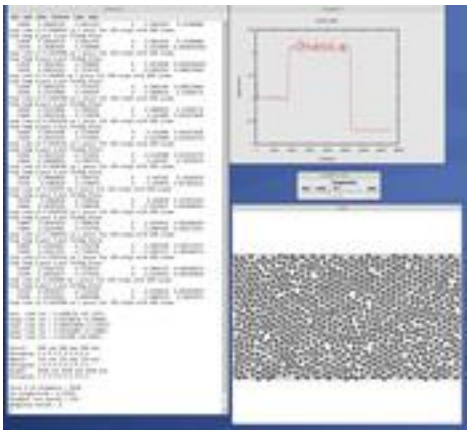
The latter link is to the open-source version.

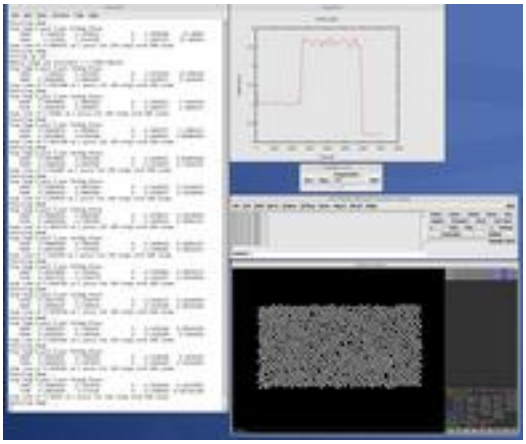
Note that for VMD, you need a fairly current version (1.8.7 works for me) and there are some lines in the pizza/vmd.py script for 4 PIZZA variables that have to match the VMD installation on your system.

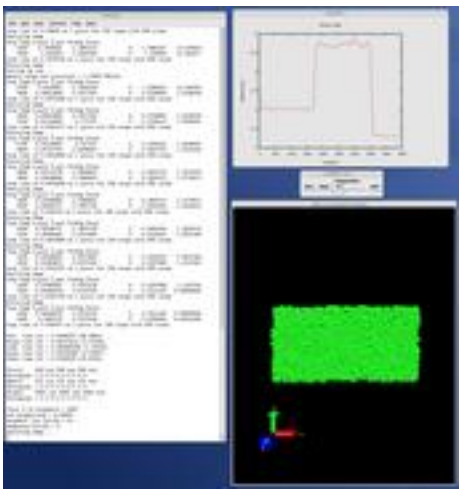
See the python/README file for instructions on how to run them and the source code for individual scripts for comments about what they do.

Here are screenshots of the vizplotgui_tool.py script in action for different visualization package options. Click to see larger images:









12.10 Call Python from a LAMMPS input script

LAMMPS has several commands which can be used to invoke Python code directly from an input script:

- *python*
- *variable python*
- *fix python/invoke*
- *pair_style python*

The *python* command which can be used to define and execute a Python function that you write the code for. The Python function can also be assigned to a LAMMPS python-style variable via the *variable* command. Each time the variable is evaluated, either in the LAMMPS input script itself, or by another LAMMPS command that uses the variable, this will trigger the Python function to be invoked.

The Python code for the function can be included directly in the input script or in an auxiliary file. The function can have arguments which are mapped to LAMMPS variables (also defined in the input script) and it can return a value to a LAMMPS variable. This is thus a mechanism for your input script to pass information to a piece of Python code, ask Python to execute the code, and return information to your input script.

Note that a Python function can be arbitrarily complex. It can import other Python modules, instantiate Python classes, call other Python functions, etc. The Python code that you provide can contain more code than the single function. It

can contain other functions or Python classes, as well as global variables or other mechanisms for storing state between calls from LAMMPS to the function.

The Python function you provide can consist of "pure" Python code that only performs operations provided by standard Python. However, the Python function can also "call back" to LAMMPS through its Python-wrapped library interface, in the manner described in the *Python run* doc page. This means it can issue LAMMPS input script commands or query and set internal LAMMPS state. As an example, this can be useful in an input script to create a more complex loop with branching logic, than can be created using the simple looping and branching logic enabled by the *next* and *if* commands.

See the *python* doc page and the *variable* doc page for its python-style variables for more info, including examples of Python code you can write for both pure Python operations and callbacks to LAMMPS.

The *fix python/invoke* command can execute Python code at selected timesteps during a simulation run.

The *pair_style python* command allows you to define pairwise potentials as python code which encodes a single pairwise interaction. This is useful for rapid development and debugging of a new potential.

To use any of these commands, you only need to build LAMMPS with the PYTHON package installed:

```
make yes-python
make machine
```

Note that this will link LAMMPS with the Python library on your system, which typically requires several auxiliary system libraries to also be linked. The list of these libraries and the paths to find them are specified in the lib/python/Makefile.lammps file. You need to insure that file contains the correct information for your version of Python and your machine to successfully build LAMMPS. See the lib/python/README file for more info.

If you want to write Python code with callbacks to LAMMPS, then you must also follow the steps summarized in the *Python run* doc page. I.e. you must build LAMMPS as a shared library and insure that Python can find the python/lammps.py file and the shared library.

If you're not familiar with Python, it's a powerful scripting and programming language which can do most everything that lower-level languages like C or C++ can do in fewer lines of code. The only drawback is slower execution speed. Python is also easy to use as a "glue" language to drive a program through its library interface, or to hook multiple pieces of software together, such as a simulation code plus a visualization tool, or to run a coupled multiscale or multiphysics model.

See the *Howto_couple* doc page for more ideas about coupling LAMMPS to other codes. See the *Howto library* doc page for a description of the LAMMPS library interface provided in src/library.h and src/library.h. That interface is exposed to Python either when calling LAMMPS from Python or when calling Python from a LAMMPS input script and then calling back to LAMMPS from Python code. The library interface is designed to be easy to add functionality to. Thus the Python interface to LAMMPS is also easy to extend as well.

If you create interesting Python scripts that run LAMMPS or interesting Python functions that can be called from a LAMMPS input script, that you think would be generally useful, please post them as a pull request to our GitHub site, and they can be added to the LAMMPS distribution or webpage.

CHAPTER

THIRTEEN

ERRORS

These doc pages describe the errors you can encounter when using LAMMPS. The common problems include conceptual issues. The messages and warnings doc pages give complete lists of all the messages the code may generate (except those generated by USER packages), with additional details for many of them.

13.1 Common problems

If two LAMMPS runs do not produce the exact same answer on different machines or different numbers of processors, this is typically not a bug. In theory you should get identical answers on any number of processors and on any machine. In practice, numerical round-off can cause slight differences and eventual divergence of molecular dynamics phase space trajectories within a few 100s or few 1000s of timesteps. However, the statistical properties of the two runs (e.g. average energy or temperature) should still be the same.

If the *velocity* command is used to set initial atom velocities, a particular atom can be assigned a different velocity when the problem is run on a different number of processors or on different machines. If this happens, the phase space trajectories of the two simulations will rapidly diverge. See the discussion of the *loop* option in the *velocity* command for details and options that avoid this issue.

Similarly, the *create_atoms* command generates a lattice of atoms. For the same physical system, the ordering and numbering of atoms by atom ID may be different depending on the number of processors.

Some commands use random number generators which may be setup to produce different random number streams on each processor and hence will produce different effects when run on different numbers of processors. A commonly-used example is the *fix langevin* command for thermostatting.

A LAMMPS simulation typically has two stages, setup and run. Most LAMMPS errors are detected at setup time; others like a bond stretching too far may not occur until the middle of a run.

LAMMPS tries to flag errors and print informative error messages so you can fix the problem. For most errors it will also print the last input script command that it was processing. Of course, LAMMPS cannot figure out your physics or numerical mistakes, like choosing too big a timestep, specifying erroneous force field coefficients, or putting 2 atoms on top of each other! If you run into errors that LAMMPS doesn't catch that you think it should flag, please send an email to the developers.

If you get an error message about an invalid command in your input script, you can determine what command is causing the problem by looking in the log.lammps file or using the *echo command* to see it on the screen. If you get an error like "Invalid … style", with … being fix, compute, pair, etc, it means that you mistyped the style name or that the command is part of an optional package which was not compiled into your executable. The list of available styles in your executable can be listed by using *the -h command-line swith*. The installation and compilation of optional packages is explained on the *Build packages* doc page.

For a given command, LAMMPS expects certain arguments in a specified order. If you mess this up, LAMMPS will often flag the error, but it may also simply read a bogus argument and assign a value that is valid, but not what you wanted. E.g. trying to read the string "abc" as an integer value of 0. Careful reading of the associated doc page for the

command should allow you to fix these problems. In most cases, where LAMMPS expects to read a number, either integer or floating point, it performs a stringent test on whether the provided input actually is an integer or floating-point number, respectively, and reject the input with an error message (for instance, when an integer is required, but a floating-point number 1.0 is provided):

```
ERROR: Expected integer parameter instead of '1.0' in input script or data file
```

Some commands allow for using variable references in place of numeric constants so that the value can be evaluated and may change over the course of a run. This is typically done with the syntax *v_name* for a parameter, where name is the name of the variable. On the other hand, immediate variable expansion with the syntax $*name* is performed while reading the input and before parsing commands,

Note: Using a variable reference (i.e. *v_name*) is only allowed if the documentation of the corresponding command explicitly says it is. Otherwise, you will receive an error message of this kind:

```
ERROR: Expected floating point parameter instead of 'v_name' in input script or data␣
↪file
```

Generally, LAMMPS will print a message to the screen and logfile and exit gracefully when it encounters a fatal error. Sometimes it will print a WARNING to the screen and logfile and continue on; you can decide if the WARNING is important or not. A WARNING message that is generated in the middle of a run is only printed to the screen, not to the logfile, to avoid cluttering up thermodynamic output. If LAMMPS crashes or hangs without spitting out an error message first then it could be a bug (see *this section*) or one of the following cases:

LAMMPS runs in the available memory a processor allows to be allocated. Most reasonable MD runs are compute limited, not memory limited, so this shouldn't be a bottleneck on most platforms. Almost all large memory allocations in the code are done via C-style malloc's which will generate an error message if you run out of memory. Smaller chunks of memory are allocated via C++ "new" statements. If you are unlucky you could run out of memory just when one of these small requests is made, in which case the code will crash or hang (in parallel), since LAMMPS doesn't trap on those errors.

Illegal arithmetic can cause LAMMPS to run slow or crash. This is typically due to invalid physics and numerics that your simulation is computing. If you see wild thermodynamic values or NaN values in your LAMMPS output, something is wrong with your simulation. If you suspect this is happening, it is a good idea to print out thermodynamic info frequently (e.g. every timestep) via the *thermo* so you can monitor what is happening. Visualizing the atom movement is also a good idea to insure your model is behaving as you expect.

In parallel, one way LAMMPS can hang is due to how different MPI implementations handle buffering of messages. If the code hangs without an error message, it may be that you need to specify an MPI setting or two (usually via an environment variable) to enable buffering or boost the sizes of messages that can be buffered.

13.2 Reporting bugs

If you are confident that you have found a bug in LAMMPS, please follow the steps outlined below:

- Check the New features and bug fixes section of the LAMMPS WWW site to see if the bug has already been addressed in a patch.
- Check that your issue can be reproduced with the latest development version of LAMMPS.
- Check the manual carefully to verify that the unexpected behavior you are observing is indeed in conflict with the documentation
- Check the GitHub Issue page if your issue has already been reported and if it is still open.

- Check the GitHub Pull Requests page if there is already a fix for your bug pending.
- Check the mailing list archives to see if the issue has been discussed before.

If none of these steps yields any useful information, please file a new bug report on the GitHub Issue page. The website will offer you to select a suitable template with explanations and then you should replace those explanations with the information that you can provide to reproduce your issue.

The most useful thing you can do to help us verify and fix a bug is to isolate the problem. Run it on the smallest number of atoms and fewest number of processors with the simplest input script that reproduces the bug. Try to identify what command or combination of commands is causing the problem and upload the complete input deck as a tar or zip archive. Please avoid using binary restart files unless the issue requires it. In the latter case you should also include an input deck to quickly generate this restart from a data file or a simple additional input.

You may also send an email to the LAMMPS mailing list at "lammps-users at lists.sourceforge.net" describing the problem with the same kind of information. The mailing list can provide a faster response, especially if the bug reported is actually expected behavior. But because of the high volume of the mailing list, it can happen that your e-mail is overlooked and then forgotten. Issues on GitHub have to be explicitly closed, so that will *guarantee* that at least one LAMMPS developer will have looked at it.

13.3 Error messages

This is an alphabetic list of the ERROR messages LAMMPS prints out and the reason why. If the explanation here is not sufficient, the documentation for the offending command may help. Error messages also list the source file and line number where the error was generated. For example, a message like this:

```
ERROR: Illegal velocity command (velocity.cpp:78)
```

means that line #78 in the file src/velocity.cpp generated the error. Looking in the source code may help you figure out what went wrong.

Note that error messages from *user-contributed packages* are not listed here. If such an error occurs and is not self-explanatory, you will need to look in the source code or contact the author of the package.

Doc page with *WARNING messages*

1-3 bond count is inconsistent An inconsistency was detected when computing the number of 1-3 neighbors for each atom. This likely means something is wrong with the bond topologies you have defined.

1-4 bond count is inconsistent An inconsistency was detected when computing the number of 1-4 neighbors for each atom. This likely means something is wrong with the bond topologies you have defined.

Accelerator sharing is not currently supported on system Multiple MPI processes cannot share the accelerator on your system. For NVIDIA GPUs, see the nvidia-smi command to change this setting.

All angle coeffs are not set All angle coefficients must be set in the data file or by the angle_coeff command before running a simulation.

All atom IDs = 0 but atom_modify id = yes Self-explanatory.

All atoms of a swapped type must have same charge. Self-explanatory.

All atoms of a swapped type must have the same charge. Self-explanatory.

All bond coeffs are not set All bond coefficients must be set in the data file or by the bond_coeff command before running a simulation.

All dihedral coeffs are not set All dihedral coefficients must be set in the data file or by the dihedral_coeff command before running a simulation.

All improper coeffs are not set All improper coefficients must be set in the data file or by the improper_coeff command before running a simulation.

All masses are not set For atom styles that define masses for each atom type, all masses must be set in the data file or by the mass command before running a simulation. They must also be set before using the velocity command.

All mol IDs should be set for fix gcmc group atoms The molecule flag is on, yet not all molecule ids in the fix group have been set to non-zero positive values by the user. This is an error since all atoms in the fix gcmc group are eligible for deletion, rotation, and translation and therefore must have valid molecule ids.

All pair coeffs are not set All pair coefficients must be set in the data file or by the pair_coeff command before running a simulation.

All read_dump x,y,z fields must be specified for scaled, triclinic coords For triclinic boxes and scaled coordinates you must specify all 3 of the x,y,z fields, else LAMMPS cannot reconstruct the unscaled coordinates.

All universe/uloop variables must have same # of values Self-explanatory.

All variables in next command must be same style Self-explanatory.

Angle atom missing in delete_bonds The delete_bonds command cannot find one or more atoms in a particular angle on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid angle.

Angle atom missing in set command The set command cannot find one or more atoms in a particular angle on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid angle.

Angle atoms %d %d %d missing on proc %d at step %ld One or more of 3 atoms needed to compute a particular angle are missing on this processor. Typically this is because the pairwise cutoff is set too short or the angle has blown apart and an atom is too far away.

Angle atoms missing on proc %d at step %ld One or more of 3 atoms needed to compute a particular angle are missing on this processor. Typically this is because the pairwise cutoff is set too short or the angle has blown apart and an atom is too far away.

Angle coeff for hybrid has invalid style Angle style hybrid uses another angle style as one of its coefficients. The angle style used in the angle_coeff command or read from a restart file is not recognized.

Angle coeffs are not set No angle coefficients have been assigned in the data file or via the angle_coeff command.

Angle extent > half of periodic box length This error was detected by the neigh_modify check yes setting. It is an error because the angle atoms are so far apart it is ambiguous how it should be defined.

Angle potential must be defined for SHAKE When shaking angles, an angle_style potential must be used.

Angle style hybrid cannot have hybrid as an argument Self-explanatory.

Angle style hybrid cannot have none as an argument Self-explanatory.

Angle style hybrid cannot use same angle style twice Self-explanatory.

Angle table must range from 0 to 180 degrees Self-explanatory.

Angle table parameters did not set N List of angle table parameters must include N setting.

Angle_coeff command before angle_style is defined Coefficients cannot be set in the data file or via the angle_coeff command until an angle_style has been assigned.

Angle_coeff command before simulation box is defined The angle_coeff command cannot be used before a read_data, read_restart, or create_box command.

Angle_coeff command when no angles allowed The chosen atom style does not allow for angles to be defined.

Angle_style command when no angles allowed The chosen atom style does not allow for angles to be defined.

Angles assigned incorrectly Angles read in from the data file were not assigned correctly to atoms. This means there is something invalid about the topology definitions.

Angles defined but no angle types The data file header lists angles but no angle types.

Append boundary must be shrink/minimum The boundary style of the face where atoms are added must be of type m (shrink/minimum).

Arccos of invalid value in variable formula Argument of arccos() must be between -1 and 1.

Arcsin of invalid value in variable formula Argument of arcsin() must be between -1 and 1.

Assigning body parameters to non-body atom Self-explanatory.

Assigning ellipsoid parameters to non-ellipsoid atom Self-explanatory.

Assigning line parameters to non-line atom Self-explanatory.

Assigning quat to non-body atom Self-explanatory.

Assigning tri parameters to non-tri atom Self-explanatory.

At least one atom of each swapped type must be present to define charges. Self-explanatory.

Atom IDs must be consecutive for velocity create loop all Self-explanatory.

Atom IDs must be used for molecular systems Atom IDs are used to identify and find partner atoms in bonds.

Atom count changed in fix neb This is not allowed in a NEB calculation.

Atom count is inconsistent, cannot write data file The sum of atoms across processors does not equal the global number of atoms. Probably some atoms have been lost.

Atom count is inconsistent, cannot write restart file Sum of atoms across processors does not equal initial total count. This is probably because you have lost some atoms.

Atom in too many rigid bodies - boost MAXBODY Fix poems has a parameter MAXBODY (in fix_poems.cpp) which determines the maximum number of rigid bodies a single atom can belong to (i.e. a multibody joint). The bodies you have defined exceed this limit.

Atom sort did not operate correctly This is an internal LAMMPS error. Please report it to the developers.

Atom style hybrid cannot have hybrid as an argument Self-explanatory.

Atom style hybrid cannot use same atom style twice Self-explanatory.

Atom style template molecule must have atom types The defined molecule(s) does not specify atom types.

Atom style was redefined after using fix property/atom This is not allowed.

Atom type must be zero in fix gcmc mol command Self-explanatory.

Atom vector in equal-style variable formula Atom vectors generate one value per atom which is not allowed in an equal-style variable.

Atom-style variable in equal-style variable formula Atom-style variables generate one value per atom which is not allowed in an equal-style variable.

Atom_modify id command after simulation box is defined The atom_modify id command cannot be used after a read_data, read_restart, or create_box command.

Atom_modify map command after simulation box is defined The atom_modify map command cannot be used after a read_data, read_restart, or create_box command.

Atom_modify sort and first options cannot be used together Self-explanatory.

Atom_style command after simulation box is defined The atom_style command cannot be used after a read_data, read_restart, or create_box command.

Atom_style line can only be used in 2d simulations Self-explanatory.

Atom_style tri can only be used in 3d simulations Self-explanatory.

Atomfile variable could not read values Check the file assigned to the variable.

Atomfile variable in equal-style variable formula Self-explanatory.

Atomfile-style variable in equal-style variable formula Self-explanatory.

Attempt to pop empty stack in fix box/relax Internal LAMMPS error. Please report it to the developers.

Attempt to push beyond stack limit in fix box/relax Internal LAMMPS error. Please report it to the developers.

Attempting to rescale a 0.0 temperature Cannot rescale a temperature that is already 0.0.

Attempting to insert more particles than available lattice points Self-explanatory.

Bad FENE bond Two atoms in a FENE bond have become so far apart that the bond cannot be computed.

Bad TIP4P angle type for PPPM/TIP4P Specified angle type is not valid.

Bad TIP4P angle type for PPPMDisp/TIP4P Specified angle type is not valid.

Bad TIP4P bond type for PPPM/TIP4P Specified bond type is not valid.

Bad TIP4P bond type for PPPMDisp/TIP4P Specified bond type is not valid.

Bad fix ID in fix append/atoms command The value of the fix_id for keyword spatial must start with 'f_'.

Bad grid of processors The 3d grid of processors defined by the processors command does not match the number of processors LAMMPS is being run on.

Bad kspace_modify kmax/ewald parameter Kspace_modify values for the kmax/ewald keyword must be integers > 0

Bad kspace_modify slab parameter Kspace_modify value for the slab/volume keyword must be >= 2.0.

Bad matrix inversion in mldivide3 This error should not occur unless the matrix is badly formed.

Bad principal moments Fix rigid did not compute the principal moments of inertia of a rigid group of atoms correctly.

Bad quadratic solve for particle/line collision This is an internal error. It should normally not occur.

Bad quadratic solve for particle/tri collision This is an internal error. It should normally not occur.

Bad real space Coulombic cutoff in fix tune/kspace Fix tune/kspace tried to find the optimal real space Coulombic cutoff using the Newton-Rhaphson method, but found a non-positive or NaN cutoff

Balance command before simulation box is defined The balance command cannot be used before a read_data, read_restart, or create_box command.

Balance produced bad splits This should not occur. It means two or more cutting plane locations are on top of each other or out of order. Report the problem to the developers.

Balance rcb cannot be used with comm_style brick Comm_style tiled must be used instead.

Balance shift string is invalid The string can only contain the characters "x", "y", or "z".

Bias compute does not calculate a velocity bias The specified compute must compute a bias for temperature.

Bias compute does not calculate temperature The specified compute must compute temperature.

Bias compute group does not match compute group The specified compute must operate on the same group as the parent compute.

Big particle in fix srd cannot be point particle Big particles must be extended spheroids or ellipsoids.

Bigint setting in lmptype.h is invalid Size of bigint is less than size of tagint.

Bigint setting in lmptype.h is not compatible Format of bigint stored in restart file is not consistent with LAMMPS version you are running. See the settings in src/lmptype.h

Bitmapped lookup tables require int/float be same size Cannot use pair tables on this machine, because of word sizes. Use the pair_modify command with table 0 instead.

Bitmapped table in file does not match requested table Setting for bitmapped table in pair_coeff command must match table in file exactly.

Bitmapped table is incorrect length in table file Number of table entries is not a correct power of 2.

Bond and angle potentials must be defined for TIP4P Cannot use TIP4P pair potential unless bond and angle potentials are defined.

Bond atom missing in box size check The 2nd atoms needed to compute a particular bond is missing on this processor. Typically this is because the pairwise cutoff is set too short or the bond has blown apart and an atom is too far away.

Bond atom missing in delete_bonds The delete_bonds command cannot find one or more atoms in a particular bond on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid bond.

Bond atom missing in image check The 2nd atom in a particular bond is missing on this processor. Typically this is because the pairwise cutoff is set too short or the bond has blown apart and an atom is too far away.

Bond atom missing in set command The set command cannot find one or more atoms in a particular bond on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid bond.

Bond atoms %d %d missing on proc %d at step %ld The 2nd atom needed to compute a particular bond is missing on this processor. Typically this is because the pairwise cutoff is set too short or the bond has blown apart and an atom is too far away.

Bond atoms missing on proc %d at step %ld The 2nd atom needed to compute a particular bond is missing on this processor. Typically this is because the pairwise cutoff is set too short or the bond has blown apart and an atom is too far away.

Bond coeff for hybrid has invalid style Bond style hybrid uses another bond style as one of its coefficients. The bond style used in the bond_coeff command or read from a restart file is not recognized.

Bond coeffs are not set No bond coefficients have been assigned in the data file or via the bond_coeff command.

Bond extent > half of periodic box length This error was detected by the neigh_modify check yes setting. It is an error because the bond atoms are so far apart it is ambiguous how it should be defined.

Bond potential must be defined for SHAKE Cannot use fix shake unless bond potential is defined.

Bond style hybrid cannot have hybrid as an argument Self-explanatory.

Bond style hybrid cannot have none as an argument Self-explanatory.

Bond style hybrid cannot use same bond style twice Self-explanatory.

Bond style quartic cannot be used with 3,4-body interactions No angle, dihedral, or improper styles can be defined when using bond style quartic.

Bond style quartic cannot be used with atom style template This bond style can change the bond topology which is not allowed with this atom style.

Bond style quartic requires special_bonds = 1,1,1 This is a restriction of the current bond quartic implementation.

Bond table parameters did not set N List of bond table parameters must include N setting.

Bond table values are not increasing The values in the tabulated file must be monotonically increasing.

BondAngle coeff for hybrid angle has invalid format No “ba” field should appear in data file entry.

BondBond coeff for hybrid angle has invalid format No “bb” field should appear in data file entry.

Bond_coeff command before bond_style is defined Coefficients cannot be set in the data file or via the bond_coeff command until an bond_style has been assigned.

Bond_coeff command before simulation box is defined The bond_coeff command cannot be used before a read_data, read_restart, or create_box command.

Bond_coeff command when no bonds allowed The chosen atom style does not allow for bonds to be defined.

Bond_style command when no bonds allowed The chosen atom style does not allow for bonds to be defined.

Bonds assigned incorrectly Bonds read in from the data file were not assigned correctly to atoms. This means there is something invalid about the topology definitions.

Bonds defined but no bond types The data file header lists bonds but no bond types.

Bond/react: Cannot use fix bond/react with non-molecular systems Only systems with bonds that can be changed can be used. Atom_style template does not qualify.

Bond/react: Invalid template atom ID in map file Atom IDs in molecule templates range from 1 to the number of atoms in the template.

Bond/react: Rmax cutoff is longer than pairwise cutoff This is not allowed because bond creation is done using the pairwise neighbor list.

Bond/react: Molecule template ID for fix bond/react does not exist A valid molecule template must have been created with the molecule command.

Bond/react: Reaction templates must contain the same number of atoms There should be a one-to-one correspondence between atoms in the pre-reacted and post-reacted templates, as specified by the map file.

Bond/react: Unknown section in map file Please ensure reaction map files are properly formatted.

Bond/react: Atom affected by reaction too close to template edge This means an atom which changes type or connectivity during the reaction is too close to an 'edge' atom defined in the superimpose file. This could cause incorrect assignment of bonds, angle, etc. Generally, this means you must include more atoms in your templates, such that there are at least two atoms between each atom involved in the reaction and an edge atom.

Bond/react: Fix bond/react needs ghost atoms from farther away This is because a processor needs to superimpose the entire unreacted molecule template onto simulation atoms it knows about. The comm_modify cutoff command can be used to extend the communication range.

Bond/react: A deleted atom cannot remain bonded to an atom that is not deleted Self-explanatory.

Bond/react: First neighbors of chiral atoms must be of mutually different types Self-explanatory.

Bond/react: Chiral atoms must have exactly four first neighbors Self-explanatory.

Bond/react: Molecule template 'Coords' section required for chiralIDs keyword The coordinates of atoms in the pre-reacted template are used to determine chirality.

Bond/react special bond generation overflow The number of special bonds per-atom created by a reaction exceeds the system setting. See the read_data or create_box command for how to specify this value.

Bond/react topology/atom exceed system topology/atom The number of bonds, angles etc per-atom created by a reaction exceeds the system setting. See the read_data or create_box command for how to specify this value.

Both restart files must use % or neither Self-explanatory.

Both restart files must use MPI-IO or neither Self-explanatory.

Both sides of boundary must be periodic Cannot specify a boundary as periodic only on the lo or hi side. Must be periodic on both sides.

Boundary command after simulation box is defined The boundary command cannot be used after a read_data, read_restart, or create_box command.

Box bounds are invalid The box boundaries specified in the read_data file are invalid. The lo value must be less than the hi value for all 3 dimensions.

Box command after simulation box is defined The box command cannot be used after a read_data, read_restart, or create_box command.

CPU neighbor lists must be used for ellipsoid/sphere mix. When using Gay-Berne or RE-squared pair styles with both ellipsoidal and spherical particles, the neighbor list must be built on the CPU

Can not specify Pxy/Pxz/Pyz in fix box/relax with non-triclinic box Only triclinic boxes can be used with off-diagonal pressure components. See the region prism command for details.

Can not specify Pxy/Pxz/Pyz in fix nvt/npt/nph with non-triclinic box Only triclinic boxes can be used with off-diagonal pressure components. See the region prism command for details.

Can only use -plog with multiple partitions Self-explanatory. See doc page discussion of command-line switches.

Can only use -pscreen with multiple partitions Self-explanatory. See doc page discussion of command-line switches.

Can only use Kokkos supported regions with Kokkos package Self-explanatory.

Can only use NEB with 1-processor replicas This is current restriction for NEB as implemented in LAMMPS.

Can only use TAD with 1-processor replicas for NEB This is current restriction for NEB as implemented in LAMMPS.

Cannot (yet) do analytic differentiation with pppm/gpu This is a current restriction of this command.

Cannot (yet) request ghost atoms with Kokkos half neighbor list This feature is not yet supported.

Cannot (yet) use 'electron' units with dipoles This feature is not yet supported.

Cannot (yet) use Ewald with triclinic box and slab correction This feature is not yet supported.

Cannot (yet) use K-space slab correction with compute group/group for triclinic systems This option is not yet supported.

Cannot (yet) use MSM with 2d simulation This feature is not yet supported.

Cannot (yet) use PPPM with triclinic box and TIP4P This feature is not yet supported.

Cannot (yet) use PPPM with triclinic box and kspace_modify diff ad This feature is not yet supported.

Cannot (yet) use PPPM with triclinic box and slab correction This feature is not yet supported.

Cannot (yet) use kspace slab correction with long-range dipoles and non-neutral systems or per-atom energy This feature is not yet supported.

Cannot (yet) use kspace_modify diff ad with compute group/group This option is not yet supported.

Cannot (yet) use kspace_style pppm/stagger with triclinic systems This feature is not yet supported.

Cannot (yet) use molecular templates with Kokkos Self-explanatory.

Cannot (yet) use respa with Kokkos Self-explanatory.

Cannot (yet) use rigid bodies with fix deform and Kokkos Self-explanatory.

Cannot (yet) use rigid bodies with fix nh and Kokkos Self-explanatory.

Cannot (yet) use single precision with MSM (remove -DFFT_SINGLE from Makefile and re-compile) Single precision cannot be used with MSM.

Cannot add atoms to fix move variable Atoms can not be added afterwards to this fix option.

Cannot append atoms to a triclinic box The simulation box must be defined with edges aligned with the Cartesian axes.

Cannot balance in z dimension for 2d simulation Self-explanatory.

Cannot change box ortho/triclinic with certain fixes defined This is because those fixes store the shape of the box. You need to use unfix to discard the fix, change the box, then redefine a new fix.

Cannot change box ortho/triclinic with dumps defined This is because some dumps store the shape of the box. You need to use undump to discard the dump, change the box, then redefine a new dump.

Cannot change box tilt factors for orthogonal box Cannot use tilt factors unless the simulation box is non-orthogonal.

Cannot change box to orthogonal when tilt is non-zero Self-explanatory.

Cannot change box z boundary to non-periodic for a 2d simulation Self-explanatory.

Cannot change dump_modify every for dump dcd The frequency of writing dump dcd snapshots cannot be changed.

Cannot change dump_modify every for dump xtc The frequency of writing dump xtc snapshots cannot be changed.

Cannot change timestep once fix srd is setup This is because various SRD properties depend on the timestep size.

Cannot change timestep with fix pour This is because fix pour pre-computes the time delay for particles to fall out of the insertion volume due to gravity.

Cannot change to comm_style brick from tiled layout Self-explanatory.

Cannot change_box after reading restart file with per-atom info This is because the restart file info cannot be migrated with the atoms. You can get around this by performing a 0-timestep run which will assign the restart file info to actual atoms.

Cannot change_box in xz or yz for 2d simulation Self-explanatory.

Cannot change_box in z dimension for 2d simulation Self-explanatory.

Cannot clear group all This operation is not allowed.

Cannot close restart file - MPI error: %s This error was generated by MPI when reading/writing an MPI-IO restart file.

Cannot compute initial g_ewald_disp LAMMPS failed to compute an initial guess for the PPPM_disp g_ewald_6 factor that partitions the computation between real space and k-space for Dispersion interactions.

Cannot create an atom map unless atoms have IDs The simulation requires a mapping from global atom IDs to local atoms, but the atoms that have been defined have no IDs.

Cannot create atoms with undefined lattice Must use the lattice command before using the create_atoms command.

Cannot create/grow a vector/array of pointers for %s LAMMPS code is making an illegal call to the templated memory allocaters, to create a vector or array of pointers.

Cannot create_atoms after reading restart file with per-atom info The per-atom info was stored to be used when by a fix that you may re-define. If you add atoms before re-defining the fix, then there will not be a correct amount of per-atom info.

Cannot create_box after simulation box is defined A simulation box can only be defined once.

Cannot currently use pair reax with pair hybrid This is not yet supported.

Cannot currently use pppm/gpu with fix balance. Self-explanatory.

Cannot delete group all Self-explanatory.

Cannot delete group currently used by a compute Self-explanatory.

Cannot delete group currently used by a dump Self-explanatory.

Cannot delete group currently used by a fix Self-explanatory.

Cannot delete group currently used by atom_modify first Self-explanatory.

Cannot delete_atoms bond yes for non-molecular systems Self-explanatory.

Cannot displace_atoms after reading restart file with per-atom info This is because the restart file info cannot be migrated with the atoms. You can get around this by performing a 0-timestep run which will assign the restart file info to actual atoms.

Cannot do GCMC on atoms in atom_modify first group This is a restriction due to the way atoms are organized in a list to enable the atom_modify first command.

Cannot do atom/swap on atoms in atom_modify first group This is a restriction due to the way atoms are organized in a list to enable the atom_modify first command.

Cannot dump sort on atom IDs with no atom IDs defined Self-explanatory.

Cannot dump sort when multiple dump files are written In this mode, each processor dumps its atoms to a file, so no sorting is allowed.

Cannot embed Python when also extending Python with LAMMPS When running LAMMPS via Python through the LAMMPS library interface you cannot also user the input script python command.

Cannot evaporate atoms in atom_modify first group This is a restriction due to the way atoms are organized in a list to enable the atom_modify first command.

Cannot find create_bonds group ID Self-explanatory.

Cannot find delete_bonds group ID Group ID used in the delete_bonds command does not exist.

Cannot find specified group ID for core particles Self-explanatory.

Cannot find specified group ID for shell particles Self-explanatory.

Cannot have both pair_modify shift and tail set to yes These 2 options are contradictory.

Cannot intersect groups using a dynamic group This operation is not allowed.

Cannot mix molecular and molecule template atom styles Self-explanatory.

Cannot open -reorder file Self-explanatory.

Cannot open ADP potential file %s The specified ADP potential file cannot be opened. Check that the path and name are correct.

Cannot open AIREBO potential file %s The specified AIREBO potential file cannot be opened. Check that the path and name are correct.

Cannot open BOP potential file %s The specified BOP potential file cannot be opened. Check that the path and name are correct.

Cannot open COMB potential file %s The specified COMB potential file cannot be opened. Check that the path and name are correct.

Cannot open COMB3 lib.comb3 file The COMB3 library file cannot be opened. Check that the path and name are correct.

Cannot open COMB3 potential file %s The specified COMB3 potential file cannot be opened. Check that the path and name are correct.

Cannot open EAM potential file %s The specified EAM potential file cannot be opened. Check that the path and name are correct.

Cannot open EIM potential file %s The specified EIM potential file cannot be opened. Check that the path and name are correct.

Cannot open LCBOP potential file %s The specified LCBOP potential file cannot be opened. Check that the path and name are correct.

Cannot open MEAM potential file %s The specified MEAM potential file cannot be opened. Check that the path and name are correct.

Cannot open SNAP coefficient file %s The specified SNAP coefficient file cannot be opened. Check that the path and name are correct.

Cannot open SNAP parameter file %s The specified SNAP parameter file cannot be opened. Check that the path and name are correct.

Cannot open Stillinger-Weber potential file %s The specified SW potential file cannot be opened. Check that the path and name are correct.

Cannot open Tersoff potential file %s The specified potential file cannot be opened. Check that the path and name are correct.

Cannot open Vashishta potential file %s The specified Vashishta potential file cannot be opened. Check that the path and name are correct.

Cannot open balance output file Self-explanatory.

Cannot open coul/streitz potential file %s The specified coul/streitz potential file cannot be opened. Check that the path and name are correct.

Cannot open custom file Self-explanatory.

Cannot open data file %s The specified file cannot be opened. Check that the path and name are correct.

Cannot open dir to search for restart file Using a "*" in the name of the restart file will open the current directory to search for matching file names.

Cannot open dump file Self-explanatory.

Cannot open dump file %s The output file for the dump command cannot be opened. Check that the path and name are correct.

Cannot open file %s The specified file cannot be opened. Check that the path and name are correct. If the file is a compressed file, also check that the gzip executable can be found and run.

Cannot open file variable file %s The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix ave/chunk file %s The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix ave/correlate file %s The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix ave/histo file %s The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix ave/time file %s The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix balance output file Self-explanatory.

Cannot open fix poems file %s The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix print file %s The output file generated by the fix print command cannot be opened

Cannot open fix qeq parameter file %s The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix qeq/comb file %s The output file for the fix qeq/combs command cannot be opened. Check that the path and name are correct.

Cannot open fix reax/bonds file %s The output file for the fix reax/bonds command cannot be opened. Check that the path and name are correct.

Cannot open fix rigid infile %s The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix rigid restart file %s The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix rigid/small infile %s The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix tmd file %s The output file for the fix tmd command cannot be opened. Check that the path and name are correct.

Cannot open fix ttm file %s The output file for the fix ttm command cannot be opened. Check that the path and name are correct.

Cannot open gzipped file LAMMPS was compiled without support for reading and writing gzipped files through a pipeline to the gzip program with -DLAMMPS_GZIP.

Cannot open input script %s Self-explanatory.

Cannot open log.cite file This file is created when you use some LAMMPS features, to indicate what paper you should cite on behalf of those who implemented the feature. Check that you have write privileges into the directory you are running in.

Cannot open log.lammps for writing The default LAMMPS log file cannot be opened. Check that the directory you are running in allows for files to be created.

Cannot open logfile The LAMMPS log file named in a command-line argument cannot be opened. Check that the path and name are correct.

Cannot open logfile %s The LAMMPS log file specified in the input script cannot be opened. Check that the path and name are correct.

Cannot open molecule file %s The specified file cannot be opened. Check that the path and name are correct.

Cannot open nb3b/harmonic potential file %s The specified potential file cannot be opened. Check that the path and name are correct.

Cannot open pair_write file The specified output file for pair energies and forces cannot be opened. Check that the path and name are correct.

Cannot open polymorphic potential file %s The specified polymorphic potential file cannot be opened. Check that the path and name are correct.

Cannot open print file %s Self-explanatory.

Cannot open processors output file Self-explanatory.

Cannot open restart file %s Self-explanatory.

Cannot open restart file for reading - MPI error: %s This error was generated by MPI when reading/writing an MPI-IO restart file.

Cannot open restart file for writing - MPI error: %s This error was generated by MPI when reading/writing an MPI-IO restart file.

Cannot open screen file The screen file specified as a command-line argument cannot be opened. Check that the directory you are running in allows for files to be created.

Cannot open temporary file for world counter. Self-explanatory.

Cannot open universe log file For a multi-partition run, the master log file cannot be opened. Check that the directory you are running in allows for files to be created.

Cannot open universe screen file For a multi-partition run, the master screen file cannot be opened. Check that the directory you are running in allows for files to be created.

Cannot read from restart file - MPI error: %s This error was generated by MPI when reading/writing an MPI-IO restart file.

Cannot read_data without add keyword after simulation box is defined Self-explanatory.

Cannot read_restart after simulation box is defined The read_restart command cannot be used after a read_data, read_restart, or create_box command.

Cannot redefine variable as a different style An equal-style variable can be re-defined but only if it was originally an equal-style variable.

Cannot replicate 2d simulation in z dimension The replicate command cannot replicate a 2d simulation in the z dimension.

Cannot replicate with fixes that store atom quantities Either fixes are defined that create and store atom-based vectors or a restart file was read which included atom-based vectors for fixes. The replicate command cannot duplicate that information for new atoms. You should use the replicate command before fixes are applied to the system.

Cannot reset timestep with a dynamic region defined Dynamic regions (see the region command) have a time dependence. Thus you cannot change the timestep when one or more of these are defined.

Cannot reset timestep with a time-dependent fix defined You cannot reset the timestep when a fix that keeps track of elapsed time is in place.

Cannot run 2d simulation with non-periodic Z dimension Use the boundary command to make the z dimension periodic in order to run a 2d simulation.

Cannot set bond topology types for atom style template The bond, angle, etc types cannot be changed for this atom style since they are static settings in the molecule template files.

Cannot set both respa pair and inner/middle/outer In the rRESPA integrator, you must compute pairwise potentials either all together (pair), or in pieces (inner/middle/outer). You can't do both.

Cannot set cutoff/multi before simulation box is defined Self-explanatory.

Cannot set dpd/theta for this atom style Self-explanatory.

Cannot set dump_modify flush for dump xtc Self-explanatory.

Cannot set mass for this atom style This atom style does not support mass settings for each atom type. Instead they are defined on a per-atom basis in the data file.

Cannot set meso/cv for this atom style Self-explanatory.

Cannot set meso/e for this atom style Self-explanatory.

Cannot set meso/rho for this atom style Self-explanatory.

Cannot set non-zero image flag for non-periodic dimension Self-explanatory.

Cannot set non-zero z velocity for 2d simulation Self-explanatory.

Cannot set quaternion for atom that has none Self-explanatory.

Cannot set quaternion with xy components for 2d system Self-explanatory.

Cannot set respa hybrid and any of pair/inner/middle/outer In the rRESPA integrator, you must compute pairwise potentials either all together (pair), with different cutoff regions (inner/middle/outer), or per hybrid sub-style (hybrid). You cannot mix those.

Cannot set respa middle without inner/outer In the rRESPA integrator, you must define both a inner and outer setting in order to use a middle setting.

Cannot set restart file size - MPI error: %s This error was generated by MPI when reading/writing an MPI-IO restart file.

Cannot set smd/contact/radius for this atom style Self-explanatory.

Cannot set smd/mass/density for this atom style Self-explanatory.

Cannot set temperature for fix rigid/nph The temp keyword cannot be specified.

Cannot set theta for atom that is not a line Self-explanatory.

Cannot set this attribute for this atom style The attribute being set does not exist for the defined atom style.

Cannot set variable z velocity for 2d simulation Self-explanatory.

Cannot skew triclinic box in z for 2d simulation Self-explanatory.

Cannot subtract groups using a dynamic group This operation is not allowed.

Cannot union groups using a dynamic group This operation is not allowed.

Cannot use -kokkos on without KOKKOS installed Self-explanatory.

Cannot use -reorder after -partition Self-explanatory. See doc page discussion of command-line switches.

Cannot use Ewald with 2d simulation The kspace style ewald cannot be used in 2d simulations. You can use 2d Ewald in a 3d simulation; see the kspace_modify command.

Cannot use Ewald/disp solver on system with no charge, dipole, or LJ particles No atoms in system have a non-zero charge or dipole, or are LJ particles. Change charges/dipoles or change options of the kspace solver/pair style.

Cannot use EwaldDisp with 2d simulation This is a current restriction of this command.

Cannot use Kokkos pair style with rRESPA inner/middle Self-explanatory.

Cannot use NEB unless atom map exists Use the atom_modify command to create an atom map.

Cannot use NEB with a single replica Self-explanatory.

Cannot use NEB with atom_modify sort enabled This is current restriction for NEB implemented in LAMMPS.

Cannot use PPPM with 2d simulation The kspace style pppm cannot be used in 2d simulations. You can use 2d PPPM in a 3d simulation; see the kspace_modify command.

Cannot use PPPMDisp with 2d simulation The kspace style pppm/disp cannot be used in 2d simulations. You can use 2d pppm/disp in a 3d simulation; see the kspace_modify command.

Cannot use PRD with a changing box The current box dimensions are not copied between replicas

Cannot use PRD with a time-dependent fix defined PRD alters the timestep in ways that will mess up these fixes.

Cannot use PRD with a time-dependent region defined PRD alters the timestep in ways that will mess up these regions.

Cannot use PRD with atom_modify sort enabled This is a current restriction of PRD. You must turn off sorting, which is enabled by default, via the atom_modify command.

Cannot use PRD with multi-processor replicas unless atom map exists Use the atom_modify command to create an atom map.

Cannot use TAD unless atom map exists for NEB See atom_modify map command to set this.

Cannot use TAD with a single replica for NEB NEB requires multiple replicas.

Cannot use TAD with atom_modify sort enabled for NEB This is a current restriction of NEB.

Cannot use a damped dynamics min style with fix box/relax This is a current restriction in LAMMPS. Use another minimizer style.

Cannot use a damped dynamics min style with per-atom DOF This is a current restriction in LAMMPS. Use another minimizer style.

Cannot use append/atoms in periodic dimension The boundary style of the face where atoms are added can not be of type p (periodic).

Cannot use atomfile-style variable unless atom map exists Self-explanatory. See the atom_modify command to create a map.

Cannot use both com and bias with compute temp/chunk Self-explanatory.

Cannot use chosen neighbor list style with buck/coul/cut/kk Self-explanatory.

Cannot use chosen neighbor list style with buck/coul/long/kk Self-explanatory.

Cannot use chosen neighbor list style with buck/kk That style is not supported by Kokkos.

Cannot use chosen neighbor list style with coul/cut/kk That style is not supported by Kokkos.

Cannot use chosen neighbor list style with coul/debye/kk Self-explanatory.

Cannot use chosen neighbor list style with coul/dsf/kk That style is not supported by Kokkos.

Cannot use chosen neighbor list style with coul/wolf/kk That style is not supported by Kokkos.

Cannot use chosen neighbor list style with lj/charmm/coul/charmm/implicit/kk Self-explanatory.

Cannot use chosen neighbor list style with lj/charmm/coul/charmm/kk Self-explanatory.

Cannot use chosen neighbor list style with lj/charmm/coul/long/kk Self-explanatory.

Cannot use chosen neighbor list style with lj/class2/coul/cut/kk Self-explanatory.

Cannot use chosen neighbor list style with lj/class2/coul/long/kk Self-explanatory.

Cannot use chosen neighbor list style with lj/class2/kk Self-explanatory.

Cannot use chosen neighbor list style with lj/cut/coul/cut/kk That style is not supported by Kokkos.

Cannot use chosen neighbor list style with lj/cut/coul/debye/kk Self-explanatory.

Cannot use chosen neighbor list style with lj/cut/coul/long/kk That style is not supported by Kokkos.

Cannot use chosen neighbor list style with lj/cut/kk That style is not supported by Kokkos.

Cannot use chosen neighbor list style with lj/expand/kk Self-explanatory.

Cannot use chosen neighbor list style with lj/gromacs/coul/gromacs/kk Self-explanatory.

Cannot use chosen neighbor list style with lj/gromacs/kk Self-explanatory.

Cannot use chosen neighbor list style with lj/sdk/kk That style is not supported by Kokkos.

Cannot use chosen neighbor list style with pair eam/kk That style is not supported by Kokkos.

Cannot use chosen neighbor list style with pair eam/kk/alloy Self-explanatory.

Cannot use chosen neighbor list style with pair eam/kk/fs Self-explanatory.

Cannot use chosen neighbor list style with pair sw/kk Self-explanatory.

Cannot use chosen neighbor list style with tersoff/kk Self-explanatory.

Cannot use chosen neighbor list style with tersoff/zbl/kk Self-explanatory.

Cannot use compute chunk/atom bin z for 2d model Self-explanatory.

Cannot use compute cluster/atom unless atoms have IDs Atom IDs are used to identify clusters.

Cannot use create_atoms rotate unless single style Self-explanatory.

Cannot use create_bonds unless atoms have IDs This command requires a mapping from global atom IDs to local atoms, but the atoms that have been defined have no IDs.

Cannot use create_bonds with non-molecular system Self-explanatory.

Cannot use cwiggle in variable formula between runs This is a function of elapsed time.

Cannot use delete_atoms bond yes with atom_style template This is because the bonds for that atom style are hard-wired in the molecule template.

Cannot use delete_atoms unless atoms have IDs Your atoms do not have IDs, so the delete_atoms command cannot be used.

Cannot use delete_bonds with non-molecular system Your choice of atom style does not have bonds.

Cannot use dump_modify fileper without % in dump file name Self-explanatory.

Cannot use dump_modify nfile without % in dump file name Self-explanatory.

Cannot use dynamic group with fix adapt atom This is not yet supported.

Cannot use fix TMD unless atom map exists Using this fix requires the ability to lookup an atom index, which is provided by an atom map. An atom map does not exist (by default) for non-molecular problems. Using the atom_modify map command will force an atom map to be created.

Cannot use fix bond/break with non-molecular systems Only systems with bonds that can be changed can be used. Atom_style template does not qualify.

Cannot use fix bond/create with non-molecular systems Only systems with bonds that can be changed can be used. Atom_style template does not qualify.

Cannot use fix bond/swap with non-molecular systems Only systems with bonds that can be changed can be used. Atom_style template does not qualify.

Cannot use fix box/relax on a 2nd non-periodic dimension When specifying an off-diagonal pressure component, the 2nd of the two dimensions must be periodic. E.g. if the xy component is specified, then the y dimension must be periodic.

Cannot use fix box/relax on a non-periodic dimension When specifying a diagonal pressure component, the dimension must be periodic.

Cannot use fix box/relax with both relaxation and scaling on a tilt factor When specifying scaling on a tilt factor component, that component can not also be controlled by the barostat. E.g. if scalexy yes is specified and also keyword tri or xy, this is wrong.

Cannot use fix box/relax with tilt factor scaling on a 2nd non-periodic dimension When specifying scaling on a tilt factor component, the 2nd of the two dimensions must be periodic. E.g. if the xy component is specified, then the y dimension must be periodic.

Cannot use fix deform on a shrink-wrapped boundary The x, y, z options cannot be applied to shrink-wrapped dimensions.

Cannot use fix deform tilt on a shrink-wrapped 2nd dim This is because the shrink-wrapping will change the value of the strain implied by the tilt factor.

Cannot use fix deform trate on a box with zero tilt The trate style alters the current strain.

Cannot use fix deposit rigid and not molecule Self-explanatory.

Cannot use fix deposit rigid and shake These two attributes are conflicting.

Cannot use fix deposit shake and not molecule Self-explanatory.

Cannot use fix enforce2d with 3d simulation Self-explanatory.

Cannot use fix gcmc in a 2d simulation Fix gcmc is set up to run in 3d only. No 2d simulations with fix gcmc are allowed.

Cannot use fix gcmc shake and not molecule Self-explanatory.

Cannot use fix msst without per-type mass defined Self-explanatory.

Cannot use fix npt and fix deform on same component of stress tensor This would be changing the same box dimension twice.

Cannot use fix nvt/npt/nph on a 2nd non-periodic dimension When specifying an off-diagonal pressure component, the 2nd of the two dimensions must be periodic. E.g. if the xy component is specified, then the y dimension must be periodic.

Cannot use fix nvt/npt/nph on a non-periodic dimension When specifying a diagonal pressure component, the dimension must be periodic.

Cannot use fix nvt/npt/nph with both xy dynamics and xy scaling Self-explanatory.

Cannot use fix nvt/npt/nph with both xz dynamics and xz scaling Self-explanatory.

Cannot use fix nvt/npt/nph with both yz dynamics and yz scaling Self-explanatory.

Cannot use fix nvt/npt/nph with xy scaling when y is non-periodic dimension The 2nd dimension in the barostatted tilt factor must be periodic.

Cannot use fix nvt/npt/nph with xz scaling when z is non-periodic dimension The 2nd dimension in the barostatted tilt factor must be periodic.

Cannot use fix nvt/npt/nph with yz scaling when z is non-periodic dimension The 2nd dimension in the barostatted tilt factor must be periodic.

Cannot use fix pour rigid and not molecule Self-explanatory.

Cannot use fix pour rigid and shake These two attributes are conflicting.

Cannot use fix pour shake and not molecule Self-explanatory.

Cannot use fix pour with triclinic box This option is not yet supported.

Cannot use fix press/berendsen and fix deform on same component of stress tensor These commands both change the box size/shape, so you cannot use both together.

Cannot use fix press/berendsen on a non-periodic dimension Self-explanatory.

Cannot use fix press/berendsen with triclinic box Self-explanatory.

Cannot use fix reax/bonds without pair_style reax Self-explanatory.

Cannot use fix rigid npt/nph and fix deform on same component of stress tensor This would be changing the same box dimension twice.

Cannot use fix rigid npt/nph on a non-periodic dimension When specifying a diagonal pressure component, the dimension must be periodic.

Cannot use fix rigid/small npt/nph on a non-periodic dimension When specifying a diagonal pressure component, the dimension must be periodic.

Cannot use fix shake with non-molecular system Your choice of atom style does not have bonds.

Cannot use fix ttm with 2d simulation This is a current restriction of this fix due to the grid it creates.

Cannot use fix ttm with triclinic box This is a current restriction of this fix due to the grid it creates.

Cannot use fix tune/kspace without a kspace style Self-explanatory.

Cannot use fix tune/kspace without a pair style This fix (tune/kspace) can only be used when a pair style has been specified.

Cannot use fix wall in periodic dimension Self-explanatory.

Cannot use fix wall zlo/zhi for a 2d simulation Self-explanatory.

Cannot use fix wall/reflect in periodic dimension Self-explanatory.

Cannot use fix wall/reflect zlo/zhi for a 2d simulation Self-explanatory.

Cannot use fix wall/srd in periodic dimension Self-explanatory.

Cannot use fix wall/srd more than once Nor is their a need to since multiple walls can be specified in one command.

Cannot use fix wall/srd without fix srd Self-explanatory.

Cannot use fix wall/srd zlo/zhi for a 2d simulation Self-explanatory.

Cannot use fix_deposit unless atoms have IDs Self-explanatory.

Cannot use fix_pour unless atoms have IDs Self-explanatory.

Cannot use include command within an if command Self-explanatory.

Cannot use lines with fix srd unless overlap is set This is because line segments are connected to each other.

Cannot use multiple fix wall commands with pair brownian Self-explanatory.

Cannot use multiple fix wall commands with pair lubricate Self-explanatory.

Cannot use multiple fix wall commands with pair lubricate/poly Self-explanatory.

Cannot use multiple fix wall commands with pair lubricateU Self-explanatory.

Cannot use neigh_modify exclude with GPU neighbor builds This is a current limitation of the GPU implementation in LAMMPS.

Cannot use neighbor bins - box size << cutoff Too many neighbor bins will be created. This typically happens when the simulation box is very small in some dimension, compared to the neighbor cutoff. Use the "nsq" style instead of "bin" style.

Cannot use newton pair with beck/gpu pair style Self-explanatory.

Cannot use newton pair with born/coul/long/gpu pair style Self-explanatory.

Cannot use newton pair with born/coul/wolf/gpu pair style Self-explanatory.

Cannot use newton pair with born/gpu pair style Self-explanatory.

Cannot use newton pair with buck/coul/cut/gpu pair style Self-explanatory.

Cannot use newton pair with buck/coul/long/gpu pair style Self-explanatory.

Cannot use newton pair with buck/gpu pair style Self-explanatory.

Cannot use newton pair with colloid/gpu pair style Self-explanatory.

Cannot use newton pair with coul/cut/gpu pair style Self-explanatory.

Cannot use newton pair with coul/debye/gpu pair style Self-explanatory.

Cannot use newton pair with coul/dsf/gpu pair style Self-explanatory.

Cannot use newton pair with coul/long/gpu pair style Self-explanatory.

Cannot use newton pair with dipole/cut/gpu pair style Self-explanatory.

Cannot use newton pair with dipole/sf/gpu pair style Self-explanatory.

Cannot use newton pair with dpd/gpu pair style Self-explanatory.

Cannot use newton pair with dpd/tstat/gpu pair style Self-explanatory.

Cannot use newton pair with eam/alloy/gpu pair style Self-explanatory.

Cannot use newton pair with eam/fs/gpu pair style Self-explanatory.

Cannot use newton pair with eam/gpu pair style Self-explanatory.

Cannot use newton pair with gauss/gpu pair style Self-explanatory.

Cannot use newton pair with gayberne/gpu pair style Self-explanatory.

Cannot use newton pair with lj/charmm/coul/long/gpu pair style Self-explanatory.

Cannot use newton pair with lj/class2/coul/long/gpu pair style Self-explanatory.

Cannot use newton pair with lj/class2/gpu pair style Self-explanatory.

Cannot use newton pair with lj/cubic/gpu pair style Self-explanatory.

Cannot use newton pair with lj/cut/coul/cut/gpu pair style Self-explanatory.

Cannot use newton pair with lj/cut/coul/debye/gpu pair style Self-explanatory.

Cannot use newton pair with lj/cut/coul/dsf/gpu pair style Self-explanatory.

Cannot use newton pair with lj/cut/coul/long/gpu pair style Self-explanatory.

Cannot use newton pair with lj/cut/coul/msm/gpu pair style Self-explanatory.

Cannot use newton pair with lj/cut/gpu pair style Self-explanatory.

Cannot use newton pair with lj/expand/gpu pair style Self-explanatory.

Cannot use newton pair with lj/gromacs/gpu pair style Self-explanatory.

Cannot use newton pair with lj/sdk/coul/long/gpu pair style Self-explanatory.

Cannot use newton pair with lj/sdk/gpu pair style Self-explanatory.

Cannot use newton pair with lj96/cut/gpu pair style Self-explanatory.

Cannot use newton pair with mie/cut/gpu pair style Self-explanatory.

Cannot use newton pair with morse/gpu pair style Self-explanatory.

Cannot use newton pair with resquared/gpu pair style Self-explanatory.

Cannot use newton pair with soft/gpu pair style Self-explanatory.

Cannot use newton pair with table/gpu pair style Self-explanatory.

Cannot use newton pair with yukawa/colloid/gpu pair style Self-explanatory.

Cannot use newton pair with yukawa/gpu pair style Self-explanatory.

Cannot use newton pair with zbl/gpu pair style Self-explanatory.

Cannot use non-zero forces in an energy minimization Fix setforce cannot be used in this manner. Use fix addforce instead.

Cannot use non-periodic boundares with fix ttm This fix requires a fully periodic simulation box.

Cannot use non-periodic boundaries with Ewald For kspace style ewald, all 3 dimensions must have periodic boundaries unless you use the kspace_modify command to define a 2d slab with a non-periodic z dimension.

Cannot use non-periodic boundaries with EwaldDisp For kspace style ewald/disp, all 3 dimensions must have periodic boundaries unless you use the kspace_modify command to define a 2d slab with a non-periodic z dimension.

Cannot use non-periodic boundaries with PPPM For kspace style pppm, all 3 dimensions must have periodic boundaries unless you use the kspace_modify command to define a 2d slab with a non-periodic z dimension.

Cannot use non-periodic boundaries with PPPMDisp For kspace style pppm/disp, all 3 dimensions must have periodic boundaries unless you use the kspace_modify command to define a 2d slab with a non-periodic z dimension.

Cannot use order greater than 8 with pppm/gpu. Self-explanatory.

Cannot use package gpu neigh yes with triclinic box This is a current restriction in LAMMPS.

Cannot use pair tail corrections with 2d simulations The correction factors are only currently defined for 3d systems.

Cannot use processors part command without using partitions See the command-line -partition switch.

Cannot use ramp in variable formula between runs This is because the ramp() function is time dependent.

Cannot use read_data add before simulation box is defined Self-explanatory.

Cannot use read_data extra with add flag Self-explanatory.

Cannot use read_data offset without add flag Self-explanatory.

Cannot use read_data shift without add flag Self-explanatory.

Cannot use region INF or EDGE when box does not exist Regions that extend to the box boundaries can only be used after the create_box command has been used.

Cannot use set atom with no atom IDs defined Atom IDs are not defined, so they cannot be used to identify an atom.

Cannot use set mol with no molecule IDs defined Self-explanatory.

Cannot use swiggle in variable formula between runs This is a function of elapsed time.

Cannot use tris with fix srd unless overlap is set This is because triangles are connected to each other.

Cannot use variable energy with constant efield in fix efield LAMMPS computes the energy itself when the E-field is constant.

Cannot use variable energy with constant force in fix addforce This is because for constant force, LAMMPS can compute the change in energy directly.

Cannot use variable every setting for dump dcd The format of DCD dump files requires snapshots be output at a constant frequency.

Cannot use variable every setting for dump xtc The format of this file requires snapshots at regular intervals.

Cannot use vdisplace in variable formula between runs This is a function of elapsed time.

Cannot use velocity bias command without temp keyword Self-explanatory.

Cannot use velocity create loop all unless atoms have IDs Atoms in the simulation to do not have IDs, so this style of velocity creation cannot be performed.

Cannot use wall in periodic dimension Self-explanatory.

Cannot use write_restart fileper without % in restart file name Self-explanatory.

Cannot use write_restart nfile without % in restart file name Self-explanatory.

Cannot wiggle and shear fix wall/gran Cannot specify both options at the same time.

Cannot write to restart file - MPI error: %s This error was generated by MPI when reading/writing an MPI-IO restart file.

Cannot yet use KSpace solver with grid with comm style tiled This is current restriction in LAMMPS.

Cannot yet use comm_style tiled with multi-mode comm Self-explanatory.

Cannot yet use comm_style tiled with triclinic box Self-explanatory.

Cannot yet use compute tally with Kokkos This feature is not yet supported.

Cannot yet use fix bond/break with this improper style This is a current restriction in LAMMPS.

Cannot yet use fix bond/create with this improper style This is a current restriction in LAMMPS.

Cannot yet use minimize with Kokkos This feature is not yet supported.

Cannot yet use pair hybrid with Kokkos This feature is not yet supported.

Cannot zero Langevin force of 0 atoms The group has zero atoms, so you cannot request its force be zeroed.

Cannot zero gld force for zero atoms There are no atoms currently in the group.

Cannot zero momentum of no atoms Self-explanatory.

Change_box command before simulation box is defined Self-explanatory.

Change_box volume used incorrectly The "dim volume" option must be used immediately following one or two settings for "dim1 ..." (and optionally "dim2 ...") and must be for a different dimension, i.e. dim != dim1 and dim != dim2.

Chunk/atom compute does not exist for compute angmom/chunk Self-explanatory.

Chunk/atom compute does not exist for compute com/chunk Self-explanatory.

Chunk/atom compute does not exist for compute gyration/chunk Self-explanatory.

Chunk/atom compute does not exist for compute inertia/chunk Self-explanatory.

Chunk/atom compute does not exist for compute msd/chunk Self-explanatory.

Chunk/atom compute does not exist for compute omega/chunk Self-explanatory.

Chunk/atom compute does not exist for compute property/chunk Self-explanatory.

Chunk/atom compute does not exist for compute temp/chunk Self-explanatory.

Chunk/atom compute does not exist for compute torque/chunk Self-explanatory.

Chunk/atom compute does not exist for compute vcm/chunk Self-explanatory.

Chunk/atom compute does not exist for fix ave/chunk Self-explanatory.

Comm tiled invalid index in box drop brick Internal error check in comm_style tiled which should not occur. Contact the developers.

Comm tiled mis-match in box drop brick Internal error check in comm_style tiled which should not occur. Contact the developers.

Comm_modify group != atom_modify first group Self-explanatory.

Communication cutoff for comm_style tiled cannot exceed periodic box length Self-explanatory.

Communication cutoff too small for SNAP micro load balancing This can happen if you change the neighbor skin after your pair_style command or if your box dimensions grow during a run. You can set the cutoff explicitly via the comm_modify cutoff command.

Compute %s does not allow use of dynamic group Dynamic groups have not yet been enabled for this compute.

Compute ID for compute chunk /atom does not exist Self-explanatory.

Compute ID for compute chunk/atom does not exist Self-explanatory.

Compute gyration ID does not exist for compute gyration/shape Self-explanatory. Provide a valid compute ID.

Compute gyration/shape compute ID does not point to a gyration compute Self-explanatory. Provide and ID of a compute gyration command.

Compute ID for compute reduce does not exist Self-explanatory.

Compute ID for compute slice does not exist Self-explanatory.

Compute ID for fix ave/atom does not exist Self-explanatory.

Compute ID for fix ave/chunk does not exist Self-explanatory.

Compute ID for fix ave/correlate does not exist Self-explanatory.

Compute ID for fix ave/histo does not exist Self-explanatory.

Compute ID for fix ave/time does not exist Self-explanatory.

Compute ID for fix store/state does not exist Self-explanatory.

Compute ID for fix vector does not exist Self-explanatory.

Compute ID must be alphanumeric or underscore characters Self-explanatory.

Compute angle/local used when angles are not allowed The atom style does not support angles.

Compute angmom/chunk does not use chunk/atom compute The style of the specified compute is not chunk/atom.

Compute body/local requires atom style body Self-explanatory.

Compute bond/local used when bonds are not allowed The atom style does not support bonds.

Compute centro/atom requires a pair style be defined This is because the computation of the centro-symmetry values uses a pairwise neighbor list.

Compute chunk/atom bin/cylinder radius is too large for periodic box Radius cannot be bigger than 1/2 of a non-axis periodic dimension.

Compute chunk/atom bin/sphere radius is too large for periodic box Radius cannot be bigger than 1/2 of any periodic dimension.

Compute chunk/atom compute array is accessed out-of-range The index for the array is out of bounds.

Compute chunk/atom compute does not calculate a per-atom array Self-explanatory.

Compute chunk/atom compute does not calculate a per-atom vector Self-explanatory.

Compute chunk/atom compute does not calculate per-atom values Self-explanatory.

Compute chunk/atom cylinder axis must be z for 2d Self-explanatory.

Compute chunk/atom fix array is accessed out-of-range the index for the array is out of bounds.

Compute chunk/atom fix does not calculate a per-atom array Self-explanatory.

Compute chunk/atom fix does not calculate a per-atom vector Self-explanatory.

Compute chunk/atom fix does not calculate per-atom values Self-explanatory.

Compute chunk/atom for triclinic boxes requires units reduced Self-explanatory.

Compute chunk/atom ids once but nchunk is not once You cannot assign chunks IDs to atom permanently if the number of chunks may change.

Compute chunk/atom molecule for non-molecular system Self-explanatory.

Compute chunk/atom sphere z origin must be 0.0 for 2d Self-explanatory.

Compute chunk/atom stores no IDs for compute property/chunk It will only store IDs if its compress option is enabled.

Compute chunk/atom stores no coord1 for compute property/chunk Only certain binning options for compute chunk/atom store coordinates.

Compute chunk/atom stores no coord2 for compute property/chunk Only certain binning options for compute chunk/atom store coordinates.

Compute chunk/atom stores no coord3 for compute property/chunk Only certain binning options for compute chunk/atom store coordinates.

Compute chunk/atom variable is not atom-style variable Self-explanatory.

Compute chunk/atom without bins cannot use discard mixed That discard option only applies to the binning styles.

Compute cluster/atom cutoff is longer than pairwise cutoff Cannot identify clusters beyond cutoff.

Compute cluster/atom requires a pair style be defined This is so that the pair style defines a cutoff distance which is used to find clusters.

Compute cna/atom cutoff is longer than pairwise cutoff Self-explanatory.

Compute cna/atom requires a pair style be defined Self-explanatory.

Compute com/chunk does not use chunk/atom compute The style of the specified compute is not chunk/atom.

Compute contact/atom requires a pair style be defined Self-explanatory.

Compute contact/atom requires atom style sphere Self-explanatory.

Compute coord/atom cutoff is longer than pairwise cutoff Cannot compute coordination at distances longer than the pair cutoff, since those atoms are not in the neighbor list.

Compute coord/atom requires a pair style be defined Self-explanatory.

Compute damage/atom requires peridynamic potential Damage is a Peridynamic-specific metric. It requires you to be running a Peridynamics simulation.

Compute dihedral/local used when dihedrals are not allowed The atom style does not support dihedrals.

Compute dilatation/atom cannot be used with this pair style Self-explanatory.

Compute dilatation/atom requires Peridynamic pair style Self-explanatory.

Compute does not allow an extra compute or fix to be reset This is an internal LAMMPS error. Please report it to the developers.

Compute erotate/asphere requires atom style ellipsoid or line or tri Self-explanatory.

Compute erotate/asphere requires extended particles This compute cannot be used with point particles.

Compute erotate/rigid with non-rigid fix-ID Self-explanatory.

Compute erotate/sphere requires atom style sphere Self-explanatory.

Compute erotate/sphere/atom requires atom style sphere Self-explanatory.

Compute event/displace has invalid fix event assigned This is an internal LAMMPS error. Please report it to the developers.

Compute group/group group ID does not exist Self-explanatory.

Compute gyration/chunk does not use chunk/atom compute The style of the specified compute is not chunk/atom.

Compute heat/flux compute ID does not compute ke/atom Self-explanatory.

Compute heat/flux compute ID does not compute pe/atom Self-explanatory.

Compute heat/flux compute ID does not compute stress/atom Self-explanatory.

Compute hexorder/atom cutoff is longer than pairwise cutoff Cannot compute order parameter beyond cutoff.

Compute hexorder/atom requires a pair style be defined Self-explanatory.

Compute improper/local used when impropers are not allowed The atom style does not support impropers.

Compute inertia/chunk does not use chunk/atom compute The style of the specified compute is not chunk/atom.

Compute ke/rigid with non-rigid fix-ID Self-explanatory.

Compute msd/chunk does not use chunk/atom compute The style of the specified compute is not chunk/atom.

Compute msd/chunk nchunk is not static This is required because the MSD cannot be computed consistently if the number of chunks is changing. Compute chunk/atom allows setting nchunk to be static.

Compute nve/asphere requires atom style ellipsoid Self-explanatory.

Compute nvt/nph/npt asphere requires atom style ellipsoid Self-explanatory.

Compute nvt/nph/npt body requires atom style body Self-explanatory.

Compute omega/chunk does not use chunk/atom compute The style of the specified compute is not chunk/atom.

Compute orientorder/atom cutoff is longer than pairwise cutoff Cannot compute order parameter beyond cutoff.

Compute orientorder/atom requires a pair style be defined Self-explanatory.

Compute pair must use group all Pair styles accumulate energy on all atoms.

Compute pe must use group all Energies computed by potentials (pair, bond, etc) are computed on all atoms.

Compute plasticity/atom cannot be used with this pair style Self-explanatory.

Compute plasticity/atom requires Peridynamic pair style Self-explanatory.

Compute pressure must use group all Virial contributions computed by potentials (pair, bond, etc) are computed on all atoms.

Compute pressure requires temperature ID to include kinetic energy The keflag cannot be used unless a temperature compute is provided.

Compute pressure temperature ID does not compute temperature The compute ID assigned to a pressure computation must compute temperature.

Compute property/atom floating point vector does not exist The command is accessing a vector added by the fix property/atom command, that does not exist.

Compute property/atom for atom property that isn't allocated Self-explanatory.

Compute property/atom integer vector does not exist The command is accessing a vector added by the fix property/atom command, that does not exist.

Compute property/chunk does not use chunk/atom compute The style of the specified compute is not chunk/atom.

Compute property/local cannot use these inputs together Only inputs that generate the same number of datums can be used together. E.g. bond and angle quantities cannot be mixed.

Compute property/local does not (yet) work with atom_style template Self-explanatory.

Compute property/local for property that isn't allocated Self-explanatory.

Compute rdf requires a pair style be defined Self-explanatory.

Compute reduce compute array is accessed out-of-range An index for the array is out of bounds.

Compute reduce compute calculates global values A compute that calculates peratom or local values is required.

Compute reduce compute does not calculate a local array Self-explanatory.

Compute reduce compute does not calculate a local vector Self-explanatory.

Compute reduce compute does not calculate a per-atom array Self-explanatory.

Compute reduce compute does not calculate a per-atom vector Self-explanatory.

Compute reduce fix array is accessed out-of-range An index for the array is out of bounds.

Compute reduce fix calculates global values A fix that calculates peratom or local values is required.

Compute reduce fix does not calculate a local array Self-explanatory.

Compute reduce fix does not calculate a local vector Self-explanatory.

Compute reduce fix does not calculate a per-atom array Self-explanatory.

Compute reduce fix does not calculate a per-atom vector Self-explanatory.

Compute reduce replace requires min or max mode Self-explanatory.

Compute reduce variable is not atom-style variable Self-explanatory.

Compute slice compute array is accessed out-of-range An index for the array is out of bounds.

Compute slice compute does not calculate a global array Self-explanatory.

Compute slice compute does not calculate a global vector Self-explanatory.

Compute slice compute does not calculate global vector or array Self-explanatory.

Compute slice compute vector is accessed out-of-range The index for the vector is out of bounds.

Compute slice fix array is accessed out-of-range An index for the array is out of bounds.

Compute slice fix does not calculate a global array Self-explanatory.

Compute slice fix does not calculate a global vector Self-explanatory.

Compute slice fix does not calculate global vector or array Self-explanatory.

Compute slice fix vector is accessed out-of-range The index for the vector is out of bounds.

Compute sna/atom cutoff is longer than pairwise cutoff Self-explanatory.

Compute sna/atom requires a pair style be defined Self-explanatory.

Compute snad/atom cutoff is longer than pairwise cutoff Self-explanatory.

Compute snad/atom requires a pair style be defined Self-explanatory.

Compute snav/atom cutoff is longer than pairwise cutoff Self-explanatory.

Compute snav/atom requires a pair style be defined Self-explanatory.

Compute stress/atom temperature ID does not compute temperature The specified compute must compute temperature.

Compute temp/asphere requires atom style ellipsoid Self-explanatory.

Compute temp/asphere requires extended particles This compute cannot be used with point particles.

Compute temp/body requires atom style body Self-explanatory.

Compute temp/body requires bodies This compute can only be applied to body particles.

Compute temp/chunk does not use chunk/atom compute The style of the specified compute is not chunk/atom.

Compute temp/cs requires ghost atoms store velocity Use the comm_modify vel yes command to enable this.

Compute temp/cs used when bonds are not allowed This compute only works on pairs of bonded particles.

Compute temp/partial cannot use vz for 2d systemx Self-explanatory.

Compute temp/profile cannot bin z for 2d systems Self-explanatory.

Compute temp/profile cannot use vz for 2d systemx Self-explanatory.

Compute temp/sphere requires atom style sphere Self-explanatory.

Compute ti kspace style does not exist Self-explanatory.

Compute ti pair style does not exist Self-explanatory.

Compute ti tail when pair style does not compute tail corrections Self-explanatory.

Compute torque/chunk does not use chunk/atom compute The style of the specified compute is not chunk/atom.

Compute used in dump between runs is not current The compute was not invoked on the current timestep, therefore it cannot be used in a dump between runs.

Compute used in variable between runs is not current Computes cannot be invoked by a variable in between runs. Thus they must have been evaluated on the last timestep of the previous run in order for their value(s) to be accessed. See the doc page for the variable command for more info.

Compute used in variable thermo keyword between runs is not current Some thermo keywords rely on a compute to calculate their value(s). Computes cannot be invoked by a variable in between runs. Thus they must have been evaluated on the last timestep of the previous run in order for their value(s) to be accessed. See the doc page for the variable command for more info.

Compute vcm/chunk does not use chunk/atom compute The style of the specified compute is not chunk/atom.

Computed temperature for fix temp/berendsen cannot be 0.0 Self-explanatory.

Computed temperature for fix temp/rescale cannot be 0.0 Cannot rescale the temperature to a new value if the current temperature is 0.0.

Core/shell partner atom not found Could not find one of the atoms in the bond pair.

Core/shell partners were not all found Could not find or more atoms in the bond pairs.

Could not adjust g_ewald_6 The Newton-Raphson solver failed to converge to a good value for g_ewald. This error should not occur for typical problems. Please send an email to the developers.

Could not compute g_ewald The Newton-Raphson solver failed to converge to a good value for g_ewald. This error should not occur for typical problems. Please send an email to the developers.

Could not compute grid size The code is unable to compute a grid size consistent with the desired accuracy. This error should not occur for typical problems. Please send an email to the developers.

Could not compute grid size for Coulomb interaction The code is unable to compute a grid size consistent with the desired accuracy. This error should not occur for typical problems. Please send an email to the developers.

Could not compute grid size for Dispersion The code is unable to compute a grid size consistent with the desired accuracy. This error should not occur for typical problems. Please send an email to the developers.

Could not create 3d FFT plan The FFT setup for the PPPM solver failed, typically due to lack of memory. This is an unusual error. Check the size of the FFT grid you are requesting.

Could not create 3d grid of processors The specified constraints did not allow a Px by Py by Pz grid to be created where Px * Py * Pz = P = total number of processors.

Could not create 3d remap plan The FFT setup in pppm failed.

Could not create Python function arguments This is an internal Python error, possibly because the number of inputs to the function is too large.

Could not create numa grid of processors The specified constraints did not allow this style of grid to be created. Usually this is because the total processor count is not a multiple of the cores/node or the user specified processor count is > 1 in one of the dimensions.

Could not create twolevel 3d grid of processors The specified constraints did not allow this style of grid to be created.

Could not evaluate Python function input variable Self-explanatory.

Could not find Python function The provided Python code was run successfully, but it not define a callable function with the required name.

Could not find atom_modify first group ID Self-explanatory.

Could not find change_box group ID Group ID used in the change_box command does not exist.

Could not find compute ID for PRD Self-explanatory.

Could not find compute ID for TAD Self-explanatory.

Could not find compute ID for temperature bias Self-explanatory.

Could not find compute ID to delete Self-explanatory.

Could not find compute displace/atom fix ID Self-explanatory.

Could not find compute event/displace fix ID Self-explanatory.

Could not find compute group ID Self-explanatory.

Could not find compute heat/flux compute ID Self-explanatory.

Could not find compute msd fix ID Self-explanatory.

Could not find compute msd/chunk fix ID The compute creates an internal fix, which has been deleted.

Could not find compute pressure temperature ID The compute ID for calculating temperature does not exist.

Could not find compute stress/atom temperature ID Self-explanatory.

Could not find compute vacf fix ID Self-explanatory.

Could not find compute/voronoi surface group ID Self-explanatory.

Could not find compute_modify ID Self-explanatory.

Could not find custom per-atom property ID Self-explanatory.

Could not find delete_atoms group ID Group ID used in the delete_atoms command does not exist.

Could not find delete_atoms region ID Region ID used in the delete_atoms command does not exist.

Could not find displace_atoms group ID Group ID used in the displace_atoms command does not exist.

Could not find dump custom compute ID Self-explanatory.

Could not find dump custom fix ID Self-explanatory.

Could not find dump custom variable name Self-explanatory.

Could not find dump group ID A group ID used in the dump command does not exist.

Could not find dump local compute ID Self-explanatory.

Could not find dump local fix ID Self-explanatory.

Could not find dump modify compute ID Self-explanatory.

Could not find dump modify custom atom floating point property ID Self-explanatory.

Could not find dump modify custom atom integer property ID Self-explanatory.

Could not find dump modify fix ID Self-explanatory.

Could not find dump modify variable name Self-explanatory.

Could not find fix ID to delete Self-explanatory.

Could not find fix adapt storage fix ID This should not happen unless you explicitly deleted a secondary fix that fix adapt created internally.

Could not find fix gcmc exclusion group ID Self-explanatory.

Could not find fix gcmc rotation group ID Self-explanatory.

Could not find fix group ID A group ID used in the fix command does not exist.

Could not find fix msst compute ID Self-explanatory.

Could not find fix poems group ID A group ID used in the fix poems command does not exist.

Could not find fix recenter group ID A group ID used in the fix recenter command does not exist.

Could not find fix rigid group ID A group ID used in the fix rigid command does not exist.

Could not find fix srd group ID Self-explanatory.

Could not find fix_modify ID A fix ID used in the fix_modify command does not exist.

Could not find fix_modify pressure ID The compute ID for computing pressure does not exist.

Could not find fix_modify temperature ID The compute ID for computing temperature does not exist.

Could not find group clear group ID Self-explanatory.

Could not find group delete group ID Self-explanatory.

Could not find pair fix ID A fix is created internally by the pair style to store shear history information. You cannot delete it.

Could not find set group ID Group ID specified in set command does not exist.

Could not find specified fix gcmc group ID Self-explanatory.

Could not find thermo compute ID Compute ID specified in thermo_style command does not exist.

Could not find thermo custom compute ID The compute ID needed by thermo style custom to compute a requested quantity does not exist.

Could not find thermo custom fix ID The fix ID needed by thermo style custom to compute a requested quantity does not exist.

Could not find thermo custom variable name Self-explanatory.

Could not find thermo fix ID Fix ID specified in thermo_style command does not exist.

Could not find thermo variable name Self-explanatory.

Could not find thermo_modify pressure ID The compute ID needed by thermo style custom to compute pressure does not exist.

Could not find thermo_modify temperature ID The compute ID needed by thermo style custom to compute temperature does not exist.

Could not find undump ID A dump ID used in the undump command does not exist.

Could not find velocity group ID A group ID used in the velocity command does not exist.

Could not find velocity temperature ID The compute ID needed by the velocity command to compute temperature does not exist.

Could not find/initialize a specified accelerator device Could not initialize at least one of the devices specified for the gpu package

Could not grab element entry from EIM potential file Self-explanatory

Could not grab global entry from EIM potential file Self-explanatory.

Could not grab pair entry from EIM potential file Self-explanatory.

Could not initialize embedded Python The main module in Python was not accessible.

Could not open Python file The specified file of Python code cannot be opened. Check that the path and name are correct.

Could not process Python file The Python code in the specified file was not run successfully by Python, probably due to errors in the Python code.

Could not process Python string The Python code in the here string was not run successfully by Python, probably due to errors in the Python code.

Coulomb PPPMDisp order has been reduced below minorder The default minimum order is 2. This can be reset by the kspace_modify minorder command.

Coulombic cutoff not supported in pair_style buck/long/coul/coul Must use long-range Coulombic interactions.

Coulombic cutoff not supported in pair_style lj/long/coul/long Must use long-range Coulombic interactions.

Coulombic cutoff not supported in pair_style lj/long/tip4p/long Must use long-range Coulombic interactions.

Coulombic cutoffs of pair hybrid sub-styles do not match If using a Kspace solver, all Coulombic cutoffs of long pair styles must be the same.

Coulombic cut not supported in pair_style lj/long/dipole/long Must use long-range Coulombic interactions.

Cound not find dump_modify ID Self-explanatory.

Create_atoms command before simulation box is defined The create_atoms command cannot be used before a read_data, read_restart, or create_box command.

Create_atoms molecule has atom IDs, but system does not The atom_style id command can be used to force atom IDs to be stored.

Create_atoms molecule must have atom types The defined molecule does not specify atom types.

Create_atoms molecule must have coordinates The defined molecule does not specify coordinates.

Create_atoms region ID does not exist A region ID used in the create_atoms command does not exist.

Create_bonds command before simulation box is defined Self-explanatory.

Create_bonds command requires no kspace_style be defined This is so that atom pairs that are already bonded to not appear in the neighbor list.

Create_bonds command requires special_bonds 1-2 weights be 0.0 This is so that atom pairs that are already bonded to not appear in the neighbor list.

Create_bonds max distance > neighbor cutoff Can only create bonds for atom pairs that will be in neighbor list.

Create_bonds requires a pair style be defined Self-explanatory.

Create_box region ID does not exist Self-explanatory.

Create_box region does not support a bounding box Not all regions represent bounded volumes. You cannot use such a region with the create_box command.

Custom floating point vector for fix store/state does not exist The command is accessing a vector added by the fix property/atom command, that does not exist.

Custom integer vector for fix store/state does not exist The command is accessing a vector added by the fix property/atom command, that does not exist.

Custom per-atom property ID is not floating point Self-explanatory.

Custom per-atom property ID is not integer Self-explanatory.

Cut-offs missing in pair_style lj/long/dipole/long Self-explanatory.

Cutoffs missing in pair_style buck/long/coul/long Self-explanatory.

Cutoffs missing in pair_style lj/long/coul/long Self-explanatory.

Cyclic loop in joint connections Fix poems cannot (yet) work with coupled bodies whose joints connect the bodies in a ring (or cycle).

Degenerate lattice primitive vectors Invalid set of 3 lattice vectors for lattice command.

Delete region ID does not exist Self-explanatory.

Delete_atoms command before simulation box is defined The delete_atoms command cannot be used before a read_data, read_restart, or create_box command.

Delete_atoms cutoff > max neighbor cutoff Can only delete atoms in atom pairs that will be in neighbor list.

Delete_atoms mol yes requires atom attribute molecule Cannot use this option with a non-molecular system.

Delete_atoms requires a pair style be defined This is because atom deletion within a cutoff uses a pairwise neighbor list.

Delete_bonds command before simulation box is defined The delete_bonds command cannot be used before a read_data, read_restart, or create_box command.

Delete_bonds command with no atoms existing No atoms are yet defined so the delete_bonds command cannot be used.

Deposition region extends outside simulation box Self-explanatory.

Did not assign all atoms correctly Atoms read in from a data file were not assigned correctly to processors. This is likely due to some atom coordinates being outside a non-periodic simulation box.

Did not assign all restart atoms correctly Atoms read in from the restart file were not assigned correctly to processors. This is likely due to some atom coordinates being outside a non-periodic simulation box. Normally this should not happen. You may wish to use the "remap" option on the read_restart command to see if this helps.

Did not find all elements in MEAM library file The requested elements were not found in the MEAM file.

Did not find fix shake partner info Could not find bond partners implied by fix shake command. This error can be triggered if the delete_bonds command was used before fix shake, and it removed bonds without resetting the 1-2, 1-3, 1-4 weighting list via the special keyword.

Did not find keyword in table file Keyword used in pair_coeff command was not found in table file.

Did not set pressure for fix rigid/nph The press keyword must be specified.

Did not set temp for fix rigid/nvt/small Self-explanatory.

Did not set temp or press for fix rigid/npt/small Self-explanatory.

Did not set temperature for fix rigid/nvt The temp keyword must be specified.

Did not set temperature or pressure for fix rigid/npt The temp and press keywords must be specified.

Dihedral atom missing in delete_bonds The delete_bonds command cannot find one or more atoms in a particular dihedral on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid dihedral.

Dihedral atom missing in set command The set command cannot find one or more atoms in a particular dihedral on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid dihedral.

Dihedral atoms %d %d %d %d missing on proc %d at step %ld One or more of 4 atoms needed to compute a particular dihedral are missing on this processor. Typically this is because the pairwise cutoff is set too short or the dihedral has blown apart and an atom is too far away.

Dihedral atoms missing on proc %d at step %ld One or more of 4 atoms needed to compute a particular dihedral are missing on this processor. Typically this is because the pairwise cutoff is set too short or the dihedral has blown apart and an atom is too far away.

Dihedral charmm is incompatible with Pair style Dihedral style charmm must be used with a pair style charmm in order for the 1-4 epsilon/sigma parameters to be defined.

Dihedral coeff for hybrid has invalid style Dihedral style hybrid uses another dihedral style as one of its coefficients. The dihedral style used in the dihedral_coeff command or read from a restart file is not recognized.

Dihedral coeffs are not set No dihedral coefficients have been assigned in the data file or via the dihedral_coeff command.

Dihedral style hybrid cannot have hybrid as an argument Self-explanatory.

Dihedral style hybrid cannot have none as an argument Self-explanatory.

Dihedral style hybrid cannot use same dihedral style twice Self-explanatory.

Dihedral/improper extent > half of periodic box length This error was detected by the neigh_modify check yes setting. It is an error because the dihedral atoms are so far apart it is ambiguous how it should be defined.

Dihedral_coeff command before dihedral_style is defined Coefficients cannot be set in the data file or via the dihedral_coeff command until an dihedral_style has been assigned.

Dihedral_coeff command before simulation box is defined The dihedral_coeff command cannot be used before a read_data, read_restart, or create_box command.

Dihedral_coeff command when no dihedrals allowed The chosen atom style does not allow for dihedrals to be defined.

Dihedral_style command when no dihedrals allowed The chosen atom style does not allow for dihedrals to be defined.

Dihedrals assigned incorrectly Dihedrals read in from the data file were not assigned correctly to atoms. This means there is something invalid about the topology definitions.

Dihedrals defined but no dihedral types The data file header lists dihedrals but no dihedral types.

Dimension command after simulation box is defined The dimension command cannot be used after a read_data, read_restart, or create_box command.

Dispersion PPPMDisp order has been reduced below minorder The default minimum order is 2. This can be reset by the kspace_modify minorder command.

Displace_atoms command before simulation box is defined The displace_atoms command cannot be used before a read_data, read_restart, or create_box command.

Distance must be > 0 for compute event/displace Self-explanatory.

Divide by 0 in influence function This should not normally occur. It is likely a problem with your model.

Divide by 0 in influence function of pair peri/lps This should not normally occur. It is likely a problem with your model.

Divide by 0 in variable formula Self-explanatory.

Domain too large for neighbor bins The domain has become extremely large so that neighbor bins cannot be used. Most likely, one or more atoms have been blown out of the simulation box to a great distance.

Double precision is not supported on this accelerator Self-explanatory

Dump atom/gz only writes compressed files The dump atom/gz output file name must have a .gz suffix.

Dump cfg arguments can not mix xs|ys|zs with xsu|ysu|zsu Self-explanatory.

Dump cfg arguments must start with 'mass type xs ys zs' or 'mass type xsu ysu zsu' This is a requirement of the CFG output format. See the dump cfg doc page for more details.

Dump cfg requires one snapshot per file Use the wildcard "*" character in the filename.

Dump cfg/gz only writes compressed files The dump cfg/gz output file name must have a .gz suffix.

Dump custom and fix not computed at compatible times The fix must produce per-atom quantities on timesteps that dump custom needs them.

Dump custom compute does not calculate per-atom array Self-explanatory.

Dump custom compute does not calculate per-atom vector Self-explanatory.

Dump custom compute does not compute per-atom info Self-explanatory.

Dump custom compute vector is accessed out-of-range Self-explanatory.

Dump custom fix does not compute per-atom array Self-explanatory.

Dump custom fix does not compute per-atom info Self-explanatory.

Dump custom fix does not compute per-atom vector Self-explanatory.

Dump custom fix vector is accessed out-of-range Self-explanatory.

Dump custom variable is not atom-style variable Only atom-style variables generate per-atom quantities, needed for dump output.

Dump custom/gz only writes compressed files The dump custom/gz output file name must have a .gz suffix.

Dump dcd of non-matching # of atoms Every snapshot written by dump dcd must contain the same # of atoms.

Dump dcd requires sorting by atom ID Use the dump_modify sort command to enable this.

Dump every variable returned a bad timestep The variable must return a timestep greater than the current timestep.

Dump file MPI-IO output not allowed with % in filename This is because a % signifies one file per processor and MPI-IO creates one large file for all processors.

Dump file does not contain requested snapshot Self-explanatory.

Dump file is incorrectly formatted Self-explanatory.

Dump image body yes requires atom style body Self-explanatory.

Dump image bond not allowed with no bond types Self-explanatory.

Dump image cannot perform sorting Self-explanatory.

Dump image line requires atom style line Self-explanatory.

Dump image persp option is not yet supported Self-explanatory.

Dump image requires one snapshot per file Use a "*" in the filename.

Dump image tri requires atom style tri Self-explanatory.

Dump local and fix not computed at compatible times The fix must produce per-atom quantities on timesteps that dump local needs them.

Dump local attributes contain no compute or fix Self-explanatory.

Dump local cannot sort by atom ID This is because dump local does not really dump per-atom info.

Dump local compute does not calculate local array Self-explanatory.

Dump local compute does not calculate local vector Self-explanatory.

Dump local compute does not compute local info Self-explanatory.

Dump local compute vector is accessed out-of-range Self-explanatory.

Dump local count is not consistent across input fields Every column of output must be the same length.

Dump local fix does not compute local array Self-explanatory.

Dump local fix does not compute local info Self-explanatory.

Dump local fix does not compute local vector Self-explanatory.

Dump local fix vector is accessed out-of-range Self-explanatory.

Dump modify bcolor not allowed with no bond types Self-explanatory.

Dump modify bdiam not allowed with no bond types Self-explanatory.

Dump modify compute ID does not compute per-atom array Self-explanatory.

Dump modify compute ID does not compute per-atom info Self-explanatory.

Dump modify compute ID does not compute per-atom vector Self-explanatory.

Dump modify compute ID vector is not large enough Self-explanatory.

Dump modify element names do not match atom types Number of element names must equal number of atom types.

Dump modify fix ID does not compute per-atom array Self-explanatory.

Dump modify fix ID does not compute per-atom info Self-explanatory.

Dump modify fix ID does not compute per-atom vector Self-explanatory.

Dump modify fix ID vector is not large enough Self-explanatory.

Dump modify variable is not atom-style variable Self-explanatory.

Dump sort column is invalid Self-explanatory.

Dump xtc requires sorting by atom ID Use the dump_modify sort command to enable this.

Dump xyz/gz only writes compressed files The dump xyz/gz output file name must have a .gz suffix.

Dump_modify buffer yes not allowed for this style Self-explanatory.

Dump_modify format string is too short There are more fields to be dumped in a line of output than your format string specifies.

Dump_modify region ID does not exist Self-explanatory.

Dumping an atom property that isn't allocated The chosen atom style does not define the per-atom quantity being dumped.

Duplicate atom IDs exist Self-explanatory.

Duplicate fields in read_dump command Self-explanatory.

Duplicate particle in PeriDynamic bond - simulation box is too small This is likely because your box length is shorter than 2 times the bond length.

Electronic temperature dropped below zero Something has gone wrong with the fix ttm electron temperature model.

Element not defined in potential file The specified element is not in the potential file.

Empty brackets in variable There is no variable syntax that uses empty brackets. Check the variable doc page.

Energy was not tallied on needed timestep You are using a thermo keyword that requires potentials to have tallied energy, but they didn't on this timestep. See the variable doc page for ideas on how to make this work.

Epsilon or sigma reference not set by pair style in PPPMDisp Self-explanatory.

Epsilon or sigma reference not set by pair style in ewald/n The pair style is not providing the needed epsilon or sigma values.

Error in vdw spline: inner radius > outer radius A pre-tabulated spline is invalid. Likely a problem with the potential parameters.

Error writing averaged chunk data Something in the output to the file triggered an error.

Error writing file header Something in the output to the file triggered an error.

Error writing out correlation data Something in the output to the file triggered an error.

Error writing out histogram data Something in the output to the file triggered an error.

Error writing out time averaged data Something in the output to the file triggered an error.

Failed to allocate %ld bytes for array %s Your LAMMPS simulation has run out of memory. You need to run a smaller simulation or on more processors.

Failed to open FFmpeg pipeline to file %s The specified file cannot be opened. Check that the path and name are correct and writable and that the FFmpeg executable can be found and run.

Failed to reallocate %ld bytes for array %s Your LAMMPS simulation has run out of memory. You need to run a smaller simulation or on more processors.

Fewer SRD bins than processors in some dimension This is not allowed. Make your SRD bin size smaller.

File variable could not read value Check the file assigned to the variable.

Final box dimension due to fix deform is < 0.0 Self-explanatory.

Fix %s does not allow use of dynamic group Dynamic groups have not yet been enabled for this fix.

Fix ID for compute chunk/atom does not exist Self-explanatory.

Fix ID for compute erotate/rigid does not exist Self-explanatory.

Fix ID for compute ke/rigid does not exist Self-explanatory.

Fix ID for compute reduce does not exist Self-explanatory.

Fix ID for compute slice does not exist Self-explanatory.

Fix ID for fix ave/atom does not exist Self-explanatory.

Fix ID for fix ave/chunk does not exist Self-explanatory.

Fix ID for fix ave/correlate does not exist Self-explanatory.

Fix ID for fix ave/histo does not exist Self-explanatory.

Fix ID for fix ave/time does not exist Self-explanatory.

Fix ID for fix store/state does not exist Self-explanatory

Fix ID for fix vector does not exist Self-explanatory.

Fix ID for read_data does not exist Self-explanatory.

Fix ID for velocity does not exist Self-explanatory.

Fix ID must be alphanumeric or underscore characters Self-explanatory.

Fix SRD: bad bin assignment for SRD advection Something has gone wrong in your SRD model; try using more conservative settings.

Fix SRD: bad search bin assignment Something has gone wrong in your SRD model; try using more conservative settings.

Fix SRD: bad stencil bin for big particle Something has gone wrong in your SRD model; try using more conservative settings.

Fix SRD: too many big particles in bin Reset the ATOMPERBIN parameter at the top of fix_srd.cpp to a larger value, and re-compile the code.

Fix SRD: too many walls in bin This should not happen unless your system has been setup incorrectly.

Fix adapt interface to this pair style not supported New coding for the pair style would need to be done.

Fix adapt kspace style does not exist Self-explanatory.

Fix adapt pair style does not exist Self-explanatory

Fix adapt pair style param not supported The pair style does not know about the parameter you specified.

Fix adapt requires atom attribute charge The atom style being used does not specify an atom charge.

Fix adapt requires atom attribute diameter The atom style being used does not specify an atom diameter.

Fix adapt type pair range is not valid for pair hybrid sub-style Self-explanatory.

Fix append/atoms requires a lattice be defined Use the lattice command for this purpose.

Fix ave/atom compute array is accessed out-of-range Self-explanatory.

Fix ave/atom compute does not calculate a per-atom array Self-explanatory.

Fix ave/atom compute does not calculate a per-atom vector A compute used by fix ave/atom must generate per-atom values.

Fix ave/atom compute does not calculate per-atom values A compute used by fix ave/atom must generate per-atom values.

Fix ave/atom fix array is accessed out-of-range Self-explanatory.

Fix ave/atom fix does not calculate a per-atom array Self-explanatory.

Fix ave/atom fix does not calculate a per-atom vector A fix used by fix ave/atom must generate per-atom values.

Fix ave/atom fix does not calculate per-atom values A fix used by fix ave/atom must generate per-atom values.

Fix ave/atom variable is not atom-style variable A variable used by fix ave/atom must generate per-atom values.

Fix ave/chunk compute does not calculate a per-atom array Self-explanatory.

Fix ave/chunk compute does not calculate a per-atom vector Self-explanatory.

Fix ave/chunk compute does not calculate per-atom values Self-explanatory.

Fix ave/chunk compute vector is accessed out-of-range Self-explanatory.

Fix ave/chunk does not use chunk/atom compute The specified compute is not for a compute chunk/atom command.

Fix ave/chunk fix does not calculate a per-atom array Self-explanatory.

Fix ave/chunk fix does not calculate a per-atom vector Self-explanatory.

Fix ave/chunk fix does not calculate per-atom values Self-explanatory.

Fix ave/chunk fix vector is accessed out-of-range Self-explanatory.

Fix ave/chunk variable is not atom-style variable Self-explanatory.

Fix ave/correlate compute does not calculate a scalar Self-explanatory.

Fix ave/correlate compute does not calculate a vector Self-explanatory.

Fix ave/correlate compute vector is accessed out-of-range The index for the vector is out of bounds.

Fix ave/correlate fix does not calculate a scalar Self-explanatory.

Fix ave/correlate fix does not calculate a vector Self-explanatory.

Fix ave/correlate fix vector is accessed out-of-range The index for the vector is out of bounds.

Fix ave/correlate variable is not equal-style variable Self-explanatory.

Fix ave/histo cannot input local values in scalar mode Self-explanatory.

Fix ave/histo cannot input per-atom values in scalar mode Self-explanatory.

Fix ave/histo compute array is accessed out-of-range Self-explanatory.

Fix ave/histo compute does not calculate a global array Self-explanatory.

Fix ave/histo compute does not calculate a global scalar Self-explanatory.

Fix ave/histo compute does not calculate a global vector Self-explanatory.

Fix ave/histo compute does not calculate a local array Self-explanatory.

Fix ave/histo compute does not calculate a local vector Self-explanatory.

Fix ave/histo compute does not calculate a per-atom array Self-explanatory.

Fix ave/histo compute does not calculate a per-atom vector Self-explanatory.

Fix ave/histo compute does not calculate local values Self-explanatory.

Fix ave/histo compute does not calculate per-atom values Self-explanatory.

Fix ave/histo compute vector is accessed out-of-range Self-explanatory.

Fix ave/histo fix array is accessed out-of-range Self-explanatory.

Fix ave/histo fix does not calculate a global array Self-explanatory.

Fix ave/histo fix does not calculate a global scalar Self-explanatory.

Fix ave/histo fix does not calculate a global vector Self-explanatory.

Fix ave/histo fix does not calculate a local array Self-explanatory.

Fix ave/histo fix does not calculate a local vector Self-explanatory.

Fix ave/histo fix does not calculate a per-atom array Self-explanatory.

Fix ave/histo fix does not calculate a per-atom vector Self-explanatory.

Fix ave/histo fix does not calculate local values Self-explanatory.

Fix ave/histo fix does not calculate per-atom values Self-explanatory.

Fix ave/histo fix vector is accessed out-of-range Self-explanatory.

Fix ave/histo input is invalid compute Self-explanatory.

Fix ave/histo input is invalid fix Self-explanatory.

Fix ave/histo input is invalid variable Self-explanatory.

Fix ave/histo inputs are not all global, peratom, or local All inputs in a single fix ave/histo command must be of the same style.

Fix ave/histo/weight value and weight vector lengths do not match Self-explanatory.

Fix ave/time cannot set output array intensive/extensive from these inputs One of more of the vector inputs has individual elements which are flagged as intensive or extensive. Such an input cannot be flagged as all intensive/extensive when turned into an array by fix ave/time.

Fix ave/time cannot use variable with vector mode Variables produce scalar values.

Fix ave/time columns are inconsistent lengths Self-explanatory.

Fix ave/time compute array is accessed out-of-range An index for the array is out of bounds.

Fix ave/time compute does not calculate a scalar Self-explanatory.

Fix ave/time compute does not calculate a vector Self-explanatory.

Fix ave/time compute does not calculate an array Self-explanatory.

Fix ave/time compute vector is accessed out-of-range The index for the vector is out of bounds.

Fix ave/time fix array cannot be variable length Self-explanatory.

Fix ave/time fix array is accessed out-of-range An index for the array is out of bounds.

Fix ave/time fix does not calculate a scalar Self-explanatory.

Fix ave/time fix does not calculate a vector Self-explanatory.

Fix ave/time fix does not calculate an array Self-explanatory.

Fix ave/time fix vector cannot be variable length Self-explanatory.

Fix ave/time fix vector is accessed out-of-range The index for the vector is out of bounds.

Fix ave/time variable is not equal-style variable Self-explanatory.

Fix balance rcb cannot be used with comm_style brick Comm_style tiled must be used instead.

Fix balance shift string is invalid The string can only contain the characters "x", "y", or "z".

Fix bond/break needs ghost atoms from further away This is because the fix needs to walk bonds to a certain distance to acquire needed info, The comm_modify cutoff command can be used to extend the communication range.

Fix bond/create angle type is invalid Self-explanatory.

Fix bond/create cutoff is longer than pairwise cutoff This is not allowed because bond creation is done using the pairwise neighbor list.

Fix bond/create dihedral type is invalid Self-explanatory.

Fix bond/create improper type is invalid Self-explanatory.

Fix bond/create induced too many angles/dihedrals/impropers per atom See the read_data command for info on using the "extra/angle/per/atom", (or dihedral, improper) keywords to allow for additional angles, dihedrals, and impropers to be formed.

Fix bond/create needs ghost atoms from further away This is because the fix needs to walk bonds to a certain distance to acquire needed info, The comm_modify cutoff command can be used to extend the communication range.

Fix bond/swap cannot use dihedral or improper styles These styles cannot be defined when using this fix.

Fix bond/swap requires pair and bond styles Self-explanatory.

Fix bond/swap requires special_bonds = 0,1,1 Self-explanatory.

Fix box/relax generated negative box length The pressure being applied is likely too large. Try applying it incrementally, to build to the high pressure.

Fix command before simulation box is defined The fix command cannot be used before a read_data, read_restart, or create_box command.

Fix deform cannot use yz variable with xy The yz setting cannot be a variable if xy deformation is also specified. This is because LAMMPS cannot determine if the yz setting will induce a box flip which would be invalid if xy is also changing.

Fix deform is changing yz too much with xy When both yz and xy are changing, it induces changes in xz if the box must flip from one tilt extreme to another. Thus it is not allowed for yz to grow so much that a flip is induced.

Fix deform tilt factors require triclinic box Cannot deform the tilt factors of a simulation box unless it is a triclinic (non-orthogonal) box.

Fix deform volume setting is invalid Cannot use volume style unless other dimensions are being controlled.

Fix deposit and fix rigid/small not using same molecule template ID Self-explanatory.

Fix deposit and fix shake not using same molecule template ID Self-explanatory.

Fix deposit molecule must have atom types The defined molecule does not specify atom types.

Fix deposit molecule must have coordinates The defined molecule does not specify coordinates.

Fix deposit molecule template ID must be same as atom_style template ID When using atom_style template, you cannot deposit molecules that are not in that template.

Fix deposit region cannot be dynamic Only static regions can be used with fix deposit.

Fix deposit region does not support a bounding box Not all regions represent bounded volumes. You cannot use such a region with the fix deposit command.

Fix deposit shake fix does not exist Self-explanatory.

Fix efield requires atom attribute q or mu The atom style defined does not have this attribute.

Fix efield with dipoles cannot use atom-style variables This option is not supported.

Fix evaporate molecule requires atom attribute molecule The atom style being used does not define a molecule ID.

Fix external callback function not set This must be done by an external program in order to use this fix.

Fix for fix ave/atom not computed at compatible time Fixes generate their values on specific timesteps. Fix ave/atom is requesting a value on a non-allowed timestep.

Fix for fix ave/chunk not computed at compatible time Fixes generate their values on specific timesteps. Fix ave/chunk is requesting a value on a non-allowed timestep.

Fix for fix ave/correlate not computed at compatible time Fixes generate their values on specific timesteps. Fix ave/correlate is requesting a value on a non-allowed timestep.

Fix for fix ave/histo not computed at compatible time Fixes generate their values on specific timesteps. Fix ave/histo is requesting a value on a non-allowed timestep.

Fix for fix ave/spatial not computed at compatible time Fixes generate their values on specific timesteps. Fix ave/spatial is requesting a value on a non-allowed timestep.

Fix for fix ave/time not computed at compatible time Fixes generate their values on specific timesteps. Fix ave/time is requesting a value on a non-allowed timestep.

Fix for fix store/state not computed at compatible time Fixes generate their values on specific timesteps. Fix store/state is requesting a value on a non-allowed timestep.

Fix for fix vector not computed at compatible time Fixes generate their values on specific timesteps. Fix vector is requesting a value on a non-allowed timestep.

Fix freeze requires atom attribute torque The atom style defined does not have this attribute.

Fix gcmc and fix shake not using same molecule template ID Self-explanatory.

Fix gcmc atom has charge, but atom style does not Self-explanatory.

Fix gcmc cannot exchange individual atoms belonging to a molecule This is an error since you should not delete only one atom of a molecule. The user has specified atomic (non-molecular) gas exchanges, but an atom belonging to a molecule could be deleted.

Fix gcmc does not (yet) work with atom_style template Self-explanatory.

Fix gcmc molecule command requires that atoms have molecule attributes Should not choose the gcmc molecule feature if no molecules are being simulated. The general molecule flag is off, but gcmc's molecule flag is on.

Fix gcmc molecule has charges, but atom style does not Self-explanatory.

Fix gcmc molecule must have atom types The defined molecule does not specify atom types.

Fix gcmc molecule must have coordinates The defined molecule does not specify coordinates.

Fix gcmc molecule template ID must be same as atom_style template ID When using atom_style template, you cannot insert molecules that are not in that template.

Fix gcmc put atom outside box This should not normally happen. Contact the developers.

Fix gcmc ran out of available atom IDs See the setting for tagint in the src/lmptype.h file.

Fix gcmc ran out of available molecule IDs See the setting for tagint in the src/lmptype.h file.

Fix gcmc region cannot be dynamic Only static regions can be used with fix gcmc.

Fix gcmc region does not support a bounding box Not all regions represent bounded volumes. You cannot use such a region with the fix gcmc command.

Fix gcmc region extends outside simulation box Self-explanatory.

Fix gcmc shake fix does not exist Self-explanatory.

Fix gld c coefficients must be >= 0 Self-explanatory.

Fix gld needs more prony series coefficients Self-explanatory.

Fix gld prony terms must be > 0 Self-explanatory.

Fix gld series type must be pprony for now Self-explanatory.

Fix gld start temperature must be >= 0 Self-explanatory.

Fix gld stop temperature must be >= 0 Self-explanatory.

Fix gld tau coefficients must be > 0 Self-explanatory.

Fix heat group has no atoms Self-explanatory.

Fix heat kinetic energy of an atom went negative This will cause the velocity rescaling about to be performed by fix heat to be invalid.

Fix heat kinetic energy went negative This will cause the velocity rescaling about to be performed by fix heat to be invalid.

Fix in variable not computed at compatible time Fixes generate their values on specific timesteps. The variable is requesting the values on a non-allowed timestep.

Fix langevin angmom is not yet implemented with kokkos This option is not yet available.

Fix langevin angmom requires atom style ellipsoid Self-explanatory.

Fix langevin angmom requires extended particles This fix option cannot be used with point particles.

Fix langevin gjf and respa are not compatible Self-explanatory.

Fix langevin gjf cannot have period equal to dt/2 If the period is equal to dt/2 then division by zero will happen.

Fix langevin gjf should come before fix nve Self-explanatory.

Fix langevin gjf with tbias is not yet implemented with kokkos This option is not yet available.

Fix langevin omega is not yet implemented with kokkos This option is not yet available.

Fix langevin omega requires atom style sphere Self-explanatory.

Fix langevin omega requires extended particles One of the particles has radius 0.0.

Fix langevin period must be > 0.0 The time window for temperature relaxation must be > 0

Fix langevin variable returned negative temperature Self-explanatory.

Fix momentum group has no atoms Self-explanatory.

Fix move cannot define z or vz variable for 2d problem Self-explanatory.

Fix move cannot rotate aroung non z-axis for 2d problem Self-explanatory.

Fix move cannot set linear z motion for 2d problem Self-explanatory.

Fix move cannot set wiggle z motion for 2d problem Self-explanatory.

Fix msst compute ID does not compute potential energy Self-explanatory.

Fix msst compute ID does not compute pressure Self-explanatory.

Fix msst compute ID does not compute temperature Self-explanatory.

Fix msst requires a periodic box Self-explanatory.

Fix msst tscale must satisfy 0 <= tscale < 1 Self-explanatory.

Fix npt/nph has tilted box too far in one step - periodic cell is too far from equilibrium state Self-explanatory. The change in the box tilt is too extreme on a short timescale.

Fix nve/asphere requires extended particles This fix can only be used for particles with a shape setting.

Fix nve/asphere/noforce requires atom style ellipsoid Self-explanatory.

Fix nve/asphere/noforce requires extended particles One of the particles is not an ellipsoid.

Fix nve/body requires atom style body Self-explanatory.

Fix nve/body requires bodies This fix can only be used for particles that are bodies.

Fix nve/line can only be used for 2d simulations Self-explanatory.

Fix nve/line requires atom style line Self-explanatory.

Fix nve/line requires line particles Self-explanatory.

Fix nve/sphere dipole requires atom attribute mu An atom style with this attribute is needed.

Fix nve/sphere requires atom style sphere Self-explanatory.

Fix nve/sphere requires extended particles This fix can only be used for particles of a finite size.

Fix nve/tri can only be used for 3d simulations Self-explanatory.

Fix nve/tri requires atom style tri Self-explanatory.

Fix nve/tri requires tri particles Self-explanatory.

Fix nvt/nph/npt asphere requires extended particles The shape setting for a particle in the fix group has shape = 0.0, which means it is a point particle.

Fix nvt/nph/npt body requires bodies Self-explanatory.

Fix nvt/nph/npt sphere requires atom style sphere Self-explanatory.

Fix nvt/npt/nph damping parameters must be > 0.0 Self-explanatory.

Fix nvt/npt/nph dilate group ID does not exist Self-explanatory.

Fix nvt/sphere requires extended particles This fix can only be used for particles of a finite size.

Fix orient/fcc file open failed The fix orient/fcc command could not open a specified file.

Fix orient/fcc file read failed The fix orient/fcc command could not read the needed parameters from a specified file.

Fix orient/fcc found self twice The neighbor lists used by fix orient/fcc are messed up. If this error occurs, it is likely a bug, so send an email to the developers.

Fix peri neigh does not exist Somehow a fix that the pair style defines has been deleted.

Fix pour and fix rigid/small not using same molecule template ID Self-explanatory.

Fix pour and fix shake not using same molecule template ID Self-explanatory.

Fix pour insertion count per timestep is 0 Self-explanatory.

Fix pour molecule must have atom types The defined molecule does not specify atom types.

Fix pour molecule must have coordinates The defined molecule does not specify coordinates.

Fix pour molecule template ID must be same as atom style template ID When using atom_style template, you cannot pour molecules that are not in that template.

Fix pour polydisperse fractions do not sum to 1.0 Self-explanatory.

Fix pour region ID does not exist Self-explanatory.

Fix pour region cannot be dynamic Only static regions can be used with fix pour.

Fix pour region does not support a bounding box Not all regions represent bounded volumes. You cannot use such a region with the fix pour command.

Fix pour requires atom attributes radius, rmass The atom style defined does not have these attributes.

Fix pour rigid fix does not exist Self-explanatory.

Fix pour shake fix does not exist Self-explanatory.

Fix press/berendsen damping parameters must be > 0.0 Self-explanatory.

Fix property/atom cannot specify mol twice Self-explanatory.

Fix property/atom cannot specify q twice Self-explanatory.

Fix property/atom mol when atom_style already has molecule attribute Self-explanatory.

Fix property/atom q when atom_style already has charge attribute Self-explanatory.

Fix property/atom vector name already exists The name for an integer or floating-point vector must be unique.

Fix qeq has negative upper Taper radius cutoff Self-explanatory.

Fix qeq/comb group has no atoms Self-explanatory.

Fix qeq/comb requires atom attribute q An atom style with charge must be used to perform charge equilibration.

Fix qeq/dynamic group has no atoms Self-explanatory.

Fix qeq/dynamic requires atom attribute q Self-explanatory.

Fix qeq/fire group has no atoms Self-explanatory.

Fix qeq/fire requires atom attribute q Self-explanatory.

Fix qeq/point group has no atoms Self-explanatory.

Fix qeq/point has insufficient QEq matrix size Occurs when number of neighbor atoms for an atom increased too much during a run. Increase SAFE_ZONE and MIN_CAP in fix_qeq.h and re-compile.

Fix qeq/point requires atom attribute q Self-explanatory.

Fix qeq/shielded group has no atoms Self-explanatory.

Fix qeq/shielded has insufficient QEq matrix size Occurs when number of neighbor atoms for an atom increased too much during a run. Increase SAFE_ZONE and MIN_CAP in fix_qeq.h and re-compile.

Fix qeq/shielded requires atom attribute q Self-explanatory.

Fix qeq/slater could not extract params from pair coul/streitz This should not happen unless pair coul/streitz has been altered.

Fix qeq/slater group has no atoms Self-explanatory.

Fix qeq/slater has insufficient QEq matrix size Occurs when number of neighbor atoms for an atom increased too much during a run. Increase SAFE_ZONE and MIN_CAP in fix_qeq.h and re-compile.

Fix qeq/slater requires atom attribute q Self-explanatory.

Fix reax/bonds numbonds > nsbmax_most The limit of the number of bonds expected by the ReaxFF force field was exceeded.

Fix recenter group has no atoms Self-explanatory.

Fix restrain requires an atom map, see atom_modify Self-explanatory.

Fix rigid atom has non-zero image flag in a non-periodic dimension Image flags for non-periodic dimensions should not be set.

Fix rigid file has no lines Self-explanatory.

Fix rigid langevin period must be > 0.0 Self-explanatory.

Fix rigid molecule requires atom attribute molecule Self-explanatory.

Fix rigid npt/nph dilate group ID does not exist Self-explanatory.

Fix rigid npt/nph does not yet allow triclinic box This is a current restriction in LAMMPS.

Fix rigid npt/nph period must be > 0.0 Self-explanatory.

Fix rigid npt/small t_chain should not be less than 1 Self-explanatory.

Fix rigid npt/small t_order must be 3 or 5 Self-explanatory.

Fix rigid nvt/npt/nph damping parameters must be > 0.0 Self-explanatory.

Fix rigid nvt/small t_chain should not be less than 1 Self-explanatory.

Fix rigid nvt/small t_iter should not be less than 1 Self-explanatory.

Fix rigid nvt/small t_order must be 3 or 5 Self-explanatory.

Fix rigid xy torque cannot be on for 2d simulation Self-explanatory.

Fix rigid z force cannot be on for 2d simulation Self-explanatory.

Fix rigid/npt period must be > 0.0 Self-explanatory.

Fix rigid/npt temperature order must be 3 or 5 Self-explanatory.

Fix rigid/npt/small period must be > 0.0 Self-explanatory.

Fix rigid/nvt period must be > 0.0 Self-explanatory.

Fix rigid/nvt temperature order must be 3 or 5 Self-explanatory.

Fix rigid/nvt/small period must be > 0.0 Self-explanatory.

Fix rigid/small atom has non-zero image flag in a non-periodic dimension Image flags for non-periodic dimensions should not be set.

Fix rigid/small langevin period must be > 0.0 Self-explanatory.

Fix rigid/small molecule must have atom types The defined molecule does not specify atom types.

Fix rigid/small molecule must have coordinates The defined molecule does not specify coordinates.

Fix rigid/small npt/nph period must be > 0.0 Self-explanatory.

Fix rigid/small nvt/npt/nph damping parameters must be > 0.0 Self-explanatory.

Fix rigid/small nvt/npt/nph dilate group ID does not exist Self-explanatory.

Fix rigid/small requires an atom map, see atom_modify Self-explanatory.

Fix rigid/small requires atom attribute molecule Self-explanatory.

Fix rigid: Bad principal moments The principal moments of inertia computed for a rigid body are not within the required tolerances.

Fix shake cannot be used with minimization Cannot use fix shake while doing an energy minimization since it turns off bonds that should contribute to the energy.

Fix shake molecule template must have shake info The defined molecule does not specify SHAKE information.

Fix spring couple group ID does not exist Self-explanatory.

Fix srd can only currently be used with comm_style brick This is a current restriction in LAMMPS.

Fix srd lamda must be >= 0.6 of SRD grid size This is a requirement for accuracy reasons.

Fix srd no-slip requires atom attribute torque This is because the SRD collisions will impart torque to the solute particles.

Fix srd requires SRD particles all have same mass Self-explanatory.

Fix srd requires ghost atoms store velocity Use the comm_modify vel yes command to enable this.

Fix srd requires newton pair on Self-explanatory.

Fix store/state compute array is accessed out-of-range Self-explanatory.

Fix store/state compute does not calculate a per-atom array The compute calculates a per-atom vector.

Fix store/state compute does not calculate a per-atom vector The compute calculates a per-atom vector.

Fix store/state compute does not calculate per-atom values Computes that calculate global or local quantities cannot be used with fix store/state.

Fix store/state fix array is accessed out-of-range Self-explanatory.

Fix store/state fix does not calculate a per-atom array The fix calculates a per-atom vector.

Fix store/state fix does not calculate a per-atom vector The fix calculates a per-atom array.

Fix store/state fix does not calculate per-atom values Fixes that calculate global or local quantities cannot be used with fix store/state.

Fix store/state for atom property that isn't allocated Self-explanatory.

Fix store/state variable is not atom-style variable Only atom-style variables calculate per-atom quantities.

Fix temp/berendsen period must be > 0.0 Self-explanatory.

Fix temp/berendsen variable returned negative temperature Self-explanatory.

Fix temp/csld is not compatible with fix rattle or fix shake These two commands cannot currently be used together with fix temp/csld.

Fix temp/csld variable returned negative temperature Self-explanatory.

Fix temp/csvr variable returned negative temperature Self-explanatory.

Fix temp/rescale variable returned negative temperature Self-explanatory.

Fix tfmc displacement length must be > 0 Self-explanatory.

Fix tfmc is not compatible with fix shake These two commands cannot currently be used together.

Fix tfmc temperature must be > 0 Self-explanatory.

Fix thermal/conductivity swap value must be positive Self-explanatory.

Fix tmd must come after integration fixes Any fix tmd command must appear in the input script after all time integration fixes (nve, nvt, npt). See the fix tmd documentation for details.

Fix ttm electron temperatures must be > 0.0 Self-explanatory.

Fix ttm electronic_density must be > 0.0 Self-explanatory.

Fix ttm electronic_specific_heat must be > 0.0 Self-explanatory.

Fix ttm electronic_thermal_conductivity must be >= 0.0 Self-explanatory.

Fix ttm gamma_p must be > 0.0 Self-explanatory.

Fix ttm gamma_s must be >= 0.0 Self-explanatory.

Fix ttm number of nodes must be > 0 Self-explanatory.

Fix ttm v_0 must be >= 0.0 Self-explanatory.

Fix used in compute chunk/atom not computed at compatible time The chunk/atom compute cannot query the output of the fix on a timestep it is needed.

Fix used in compute reduce not computed at compatible time Fixes generate their values on specific timesteps. Compute reduce is requesting a value on a non-allowed timestep.

Fix used in compute slice not computed at compatible time Fixes generate their values on specific timesteps. Compute slice is requesting a value on a non-allowed timestep.

Fix vector cannot set output array intensive/extensive from these inputs The inputs to the command have conflicting intensive/extensive attributes. You need to use more than one fix vector command.

Fix vector compute does not calculate a scalar Self-explanatory.

Fix vector compute does not calculate a vector Self-explanatory.

Fix vector compute vector is accessed out-of-range Self-explanatory.

Fix vector fix does not calculate a scalar Self-explanatory.

Fix vector fix does not calculate a vector Self-explanatory.

Fix vector fix vector is accessed out-of-range Self-explanatory.

Fix vector variable is not equal-style variable Self-explanatory.

Fix viscosity swap value must be positive Self-explanatory.

Fix viscosity vtarget value must be positive Self-explanatory.

Fix wall cutoff <= 0.0 Self-explanatory.

Fix wall/colloid requires atom style sphere Self-explanatory.

Fix wall/colloid requires extended particles One of the particles has radius 0.0.

Fix wall/gran is incompatible with Pair style Must use a granular pair style to define the parameters needed for this fix.

Fix wall/gran requires atom style sphere Self-explanatory.

Fix wall/piston command only available at zlo The face keyword must be zlo.

Fix wall/region colloid requires atom style sphere Self-explanatory.

Fix wall/region colloid requires extended particles One of the particles has radius 0.0.

Fix wall/region cutoff <= 0.0 Self-explanatory.

Fix_modify pressure ID does not compute pressure The compute ID assigned to the fix must compute pressure.

Fix_modify temperature ID does not compute temperature The compute ID assigned to the fix must compute temperature.

For triclinic deformation, specified target stress must be hydrostatic Triclinic pressure control is allowed using the tri keyword, but non-hydrostatic pressure control can not be used in this case.

Found no restart file matching pattern When using a "*" in the restart file name, no matching file was found.

GPU library not compiled for this accelerator Self-explanatory.

GPU package does not (yet) work with atom_style template Self-explanatory.

GPU particle split must be set to 1 for this pair style. For this pair style, you cannot run part of the force calculation on the host. See the package command.

GPUs are requested but Kokkos has not been compiled for CUDA Re-compile Kokkos with CUDA support to use GPUs.

Ghost velocity forward comm not yet implemented with Kokkos This is a current restriction.

Gmask function in equal-style variable formula Gmask is per-atom operation.

Gravity changed since fix pour was created The gravity vector defined by fix gravity must be static.

Gravity must point in -y to use with fix pour in 2d Self-explanatory.

Gravity must point in -z to use with fix pour in 3d Self-explanatory.

Grmask function in equal-style variable formula Grmask is per-atom operation.

Group ID does not exist A group ID used in the group command does not exist.

Group ID in variable formula does not exist Self-explanatory.

Group all cannot be made dynamic This operation is not allowed.

Group command before simulation box is defined The group command cannot be used before a read_data, read_restart, or create_box command.

Group dynamic cannot reference itself Self-explanatory.

Group dynamic parent group cannot be dynamic Self-explanatory.

Group dynamic parent group does not exist Self-explanatory.

Group region ID does not exist A region ID used in the group command does not exist.

If read_dump purges it cannot replace or trim These operations are not compatible. See the read_dump doc page for details.

Illegal ... command Self-explanatory. Check the input script syntax and compare to the documentation for the command. You can use -echo screen as a command-line option when running LAMMPS to see the offending line.

Illegal COMB parameter One or more of the coefficients defined in the potential file is invalid.

Illegal COMB3 parameter One or more of the coefficients defined in the potential file is invalid.

Illegal Stillinger-Weber parameter One or more of the coefficients defined in the potential file is invalid.

Illegal Tersoff parameter One or more of the coefficients defined in the potential file is invalid.

Illegal Vashishta parameter One or more of the coefficients defined in the potential file is invalid.

Illegal compute voronoi/atom command (occupation and (surface or edges)) Self-explanatory.

Illegal coul/streitz parameter One or more of the coefficients defined in the potential file is invalid.

Illegal dump_modify sfactor value (must be > 0.0) Self-explanatory.

Illegal dump_modify tfactor value (must be > 0.0) Self-explanatory.

Illegal fix gcmc gas mass <= 0 The computed mass of the designated gas molecule or atom type was less than or equal to zero.

Illegal fix tfmc random seed Seeds can only be nonzero positive integers.

Illegal fix wall/piston velocity The piston velocity must be positive.

Illegal integrate style Self-explanatory.

Illegal nb3b/harmonic parameter One or more of the coefficients defined in the potential file is invalid.

Illegal number of angle table entries There must be at least 2 table entries.

Illegal number of bond table entries There must be at least 2 table entries.

Illegal number of pair table entries There must be at least 2 table entries.

Illegal or unset periodicity in restart This error should not normally occur unless the restart file is invalid.

Illegal range increment value The increment must be >= 1.

Illegal simulation box The lower bound of the simulation box is greater than the upper bound.

Illegal size double vector read requested This error should not normally occur unless the restart file is invalid.

Illegal size integer vector read requested This error should not normally occur unless the restart file is invalid.

Illegal size string or corrupt restart This error should not normally occur unless the restart file is invalid.

Imageint setting in lmptype.h is invalid Imageint must be as large or larger than smallint.

Imageint setting in lmptype.h is not compatible Format of imageint stored in restart file is not consistent with LAMMPS version you are running. See the settings in src/lmptype.h

Improper atom missing in delete_bonds The delete_bonds command cannot find one or more atoms in a particular improper on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid improper.

Improper atom missing in set command The set command cannot find one or more atoms in a particular improper on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid improper.

Improper atoms %d %d %d %d missing on proc %d at step %ld One or more of 4 atoms needed to compute a particular improper are missing on this processor. Typically this is because the pairwise cutoff is set too short or the improper has blown apart and an atom is too far away.

Improper atoms missing on proc %d at step %ld One or more of 4 atoms needed to compute a particular improper are missing on this processor. Typically this is because the pairwise cutoff is set too short or the improper has blown apart and an atom is too far away.

Improper coeff for hybrid has invalid style Improper style hybrid uses another improper style as one of its coefficients. The improper style used in the improper_coeff command or read from a restart file is not recognized.

Improper coeffs are not set No improper coefficients have been assigned in the data file or via the improper_coeff command.

Improper style hybrid cannot have hybrid as an argument Self-explanatory.

Improper style hybrid cannot have none as an argument Self-explanatory.

Improper style hybrid cannot use same improper style twice Self-explanatory.

Improper_coeff command before improper_style is defined Coefficients cannot be set in the data file or via the improper_coeff command until an improper_style has been assigned.

Improper_coeff command before simulation box is defined The improper_coeff command cannot be used before a read_data, read_restart, or create_box command.

Improper_coeff command when no impropers allowed The chosen atom style does not allow for impropers to be defined.

Improper_style command when no impropers allowed The chosen atom style does not allow for impropers to be defined.

Impropers assigned incorrectly Impropers read in from the data file were not assigned correctly to atoms. This means there is something invalid about the topology definitions.

Impropers defined but no improper types The data file header lists improper but no improper types.

Incompatible KIM Simulator Model The requested KIM Simulator Model was defined for a different MD code and thus is not compatible with LAMMPS.

Incompatible units for KIM Simulator Model The selected unit style is not compatible with the requested KIM Simulator Model.

Incomplete use of variables in create_atoms command The var and set options must be used together.

Inconsistent iparam/jparam values in fix bond/create command If itype and jtype are the same, then their maxbond and newtype settings must also be the same.

Inconsistent line segment in data file The end points of the line segment are not equal distances from the center point which is the atom coordinate.

Inconsistent triangle in data file The centroid of the triangle as defined by the corner points is not the atom coordinate.

Inconsistent use of finite-size particles by molecule template molecules Not all of the molecules define a radius for their constituent particles.

Incorrect # of floating-point values in Bodies section of data file See doc page for body style.

Incorrect # of integer values in Bodies section of data file See doc page for body style.

Incorrect %s format in data file A section of the data file being read by fix property/atom does not have the correct number of values per line.

Incorrect SNAP parameter file The file cannot be parsed correctly, check its internal syntax.

Incorrect args for angle coefficients Self-explanatory. Check the input script or data file.

Incorrect args for bond coefficients Self-explanatory. Check the input script or data file.

Incorrect args for dihedral coefficients Self-explanatory. Check the input script or data file.

Incorrect args for improper coefficients Self-explanatory. Check the input script or data file.

Incorrect args for pair coefficients Self-explanatory. Check the input script or data file.

Incorrect args in pair_style command Self-explanatory.

Incorrect atom format in data file Number of values per atom line in the data file is not consistent with the atom style.

Incorrect atom format in neb file The number of fields per line is not what expected.

Incorrect bonus data format in data file See the read_data doc page for a description of how various kinds of bonus data must be formatted for certain atom styles.

Incorrect boundaries with slab Ewald Must have periodic x,y dimensions and non-periodic z dimension to use 2d slab option with Ewald.

Incorrect boundaries with slab EwaldDisp Must have periodic x,y dimensions and non-periodic z dimension to use 2d slab option with Ewald.

Incorrect boundaries with slab PPPM Must have periodic x,y dimensions and non-periodic z dimension to use 2d slab option with PPPM.

Incorrect boundaries with slab PPPMDisp Must have periodic x,y dimensions and non-periodic z dimension to use 2d slab option with pppm/disp.

Incorrect conversion in format string A format style variable was not using either a %f, a %g, or a %e conversion. Or an immediate variable with format suffix was not using either a %f, a %g or a %e conversion in the format suffix.

Incorrect element names in ADP potential file The element names in the ADP file do not match those requested.

Incorrect element names in EAM potential file The element names in the EAM file do not match those requested.

Incorrect format of ... section in data file Number or type of values per line in the given section of the data file is not consistent with the requirements for this section.

Incorrect format in COMB potential file Incorrect number of words per line in the potential file.

Incorrect format in COMB3 potential file Incorrect number of words per line in the potential file.

Incorrect format in MEAM potential file Incorrect number of words per line in the potential file.

Incorrect format in SNAP coefficient file Incorrect number of words per line in the coefficient file.

Incorrect format in SNAP parameter file Incorrect number of words per line in the parameter file.

Incorrect format in Stillinger-Weber potential file Incorrect number of words per line in the potential file.

Incorrect format in TMD target file Format of file read by fix tmd command is incorrect.

Incorrect format in Tersoff potential file Incorrect number of words per line in the potential file.

Incorrect format in Vashishta potential file Incorrect number of words per line in the potential file.

Incorrect format in coul/streitz potential file Incorrect number of words per line in the potential file.

Incorrect format in nb3b/harmonic potential file Incorrect number of words per line in the potential file.

Incorrect integer value in Bodies section of data file See doc page for body style.

Incorrect multiplicity arg for dihedral coefficients Self-explanatory. Check the input script or data file.

Incorrect number of elements in potential file Self-explanatory.

Incorrect rigid body format in fix rigid file The number of fields per line is not what expected.

Incorrect rigid body format in fix rigid/small file The number of fields per line is not what expected.

Incorrect sign arg for dihedral coefficients Self-explanatory. Check the input script or data file.

Incorrect table format check for element types Self-explanatory.

Incorrect velocity format in data file Each atom style defines a format for the Velocity section of the data file. The read-in lines do not match.

Incorrect weight arg for dihedral coefficients Self-explanatory. Check the input script or data file.

Index between variable brackets must be positive Self-explanatory.

Indexed per-atom vector in variable formula without atom map Accessing a value from an atom vector requires the ability to lookup an atom index, which is provided by an atom map. An atom map does not exist (by default) for non-molecular problems. Using the atom_modify map command will force an atom map to be created.

Initial temperatures not all set in fix ttm Self-explanatory.

Input line quote not followed by white-space An end quote must be followed by white-space.

Insertion region extends outside simulation box Self-explanatory.

Insufficient Jacobi rotations for POEMS body Eigensolve for rigid body was not sufficiently accurate.

Insufficient Jacobi rotations for body nparticle Eigensolve for rigid body was not sufficiently accurate.

Insufficient Jacobi rotations for rigid body Eigensolve for rigid body was not sufficiently accurate.

Insufficient Jacobi rotations for rigid molecule Eigensolve for rigid body was not sufficiently accurate.

Insufficient Jacobi rotations for triangle The calculation of the inertia tensor of the triangle failed. This should not happen if it is a reasonably shaped triangle.

Insufficient memory on accelerator There is insufficient memory on one of the devices specified for the gpu package

Internal error in atom_style body This error should not occur. Contact the developers.

Invalid -reorder N value Self-explanatory.

Invalid Angles section in molecule file Self-explanatory.

Invalid Bonds section in molecule file Self-explanatory.

Invalid Boolean syntax in if command Self-explanatory.

Invalid Charges section in molecule file Self-explanatory.

Invalid Coords section in molecule file Self-explanatory.

Invalid Diameters section in molecule file Self-explanatory.

Invalid Dihedrals section in molecule file Self-explanatory.

Invalid Impropers section in molecule file Self-explanatory.

Invalid Kokkos command-line args Self-explanatory. See Section 2.7 of the manual for details.

Invalid LAMMPS restart file The file does not appear to be a LAMMPS restart file since it doesn't contain the correct magic string at the beginning.

Invalid Masses section in molecule file Self-explanatory.

Invalid REAX atom type There is a mis-match between LAMMPS atom types and the elements listed in the ReaxFF force field file.

Invalid Special Bond Counts section in molecule file Self-explanatory.

Invalid Types section in molecule file Self-explanatory.

Invalid angle count in molecule file Self-explanatory.

Invalid angle table length Length must be 2 or greater.

Invalid angle type in Angles section of data file Angle type must be positive integer and within range of specified angle types.

Invalid angle type in Angles section of molecule file Self-explanatory.

Invalid angle type index for fix shake Self-explanatory.

Invalid args for non-hybrid pair coefficients "NULL" is only supported in pair_coeff calls when using pair hybrid

Invalid argument to factorial %d N must be >= 0 and <= 167, otherwise the factorial result is too large.

Invalid atom ID in %s section of data file An atom in a section of the data file being read by fix property/atom has an invalid atom ID that is <= 0 or > the maximum existing atom ID.

Invalid atom ID in Angles section of data file Atom IDs must be positive integers and within range of defined atoms.

Invalid atom ID in Angles section of molecule file Self-explanatory.

Invalid atom ID in Atoms section of data file Atom IDs must be positive integers.

Invalid atom ID in Bodies section of data file Atom IDs must be positive integers and within range of defined atoms.

Invalid atom ID in Bonds section of data file Atom IDs must be positive integers and within range of defined atoms.

Invalid atom ID in Bonds section of molecule file Self-explanatory.

Invalid atom ID in Bonus section of data file Atom IDs must be positive integers and within range of defined atoms.

Invalid atom ID in Dihedrals section of data file Atom IDs must be positive integers and within range of defined atoms.

Invalid atom ID in Impropers section of data file Atom IDs must be positive integers and within range of defined atoms.

Invalid atom ID in Velocities section of data file Atom IDs must be positive integers and within range of defined atoms.

Invalid atom ID in dihedrals section of molecule file Self-explanatory.

Invalid atom ID in impropers section of molecule file Self-explanatory.

Invalid atom ID in variable file Self-explanatory.

Invalid atom IDs in neb file An ID in the file was not found in the system.

Invalid atom diameter in molecule file Diameters must be >= 0.0.

Invalid atom mass for fix shake Mass specified in fix shake command must be > 0.0.

Invalid atom mass in molecule file Masses must be > 0.0.

Invalid atom type in Atoms section of data file Atom types must range from 1 to specified # of types.

Invalid atom type in create_atoms command The create_box command specified the range of valid atom types. An invalid type is being requested.

Invalid atom type in create_atoms mol command The atom types in the defined molecule are added to the value specified in the create_atoms command, as an offset. The final value for each atom must be between 1 to N, where N is the number of atom types.

Invalid atom type in fix atom/swap command The atom type specified in the atom/swap command does not exist.

Invalid atom type in fix bond/create command Self-explanatory.

Invalid atom type in fix deposit command Self-explanatory.

Invalid atom type in fix deposit mol command The atom types in the defined molecule are added to the value specified in the create_atoms command, as an offset. The final value for each atom must be between 1 to N, where N is the number of atom types.

Invalid atom type in fix gcmc command The atom type specified in the gcmc command does not exist.

Invalid atom type in fix pour command Self-explanatory.

Invalid atom type in fix pour mol command The atom types in the defined molecule are added to the value specified in the create_atoms command, as an offset. The final value for each atom must be between 1 to N, where N is the number of atom types.

Invalid atom type in molecule file Atom types must range from 1 to specified # of types.

Invalid atom type in neighbor exclusion list Atom types must range from 1 to Ntypes inclusive.

Invalid atom type index for fix shake Atom types must range from 1 to Ntypes inclusive.

Invalid atom types in pair_write command Atom types must range from 1 to Ntypes inclusive.

Invalid atom vector in variable formula The atom vector is not recognized.

Invalid atom_style body command No body style argument was provided.

Invalid atom_style command Self-explanatory.

Invalid attribute in dump custom command Self-explanatory.

Invalid attribute in dump local command Self-explanatory.

Invalid attribute in dump modify command Self-explanatory.

Invalid basis setting in create_atoms command The basis index must be between 1 to N where N is the number of basis atoms in the lattice. The type index must be between 1 to N where N is the number of atom types.

Invalid basis setting in fix append/atoms command The basis index must be between 1 to N where N is the number of basis atoms in the lattice. The type index must be between 1 to N where N is the number of atom types.

Invalid bin bounds in compute chunk/atom The lo/hi values are inconsistent.

Invalid bin bounds in fix ave/spatial The lo/hi values are inconsistent.

Invalid body nparticle command Arguments in atom-style command are not correct.

Invalid bond count in molecule file Self-explanatory.

Invalid bond table length Length must be 2 or greater.

Invalid bond type in Bonds section of data file Bond type must be positive integer and within range of specified bond types.

Invalid bond type in Bonds section of molecule file Self-explanatory.

Invalid bond type in create_bonds command Self-explanatory.

Invalid bond type in fix bond/break command Self-explanatory.

Invalid bond type in fix bond/create command Self-explanatory.

Invalid bond type index for fix shake Self-explanatory. Check the fix shake command in the input script.

Invalid coeffs for this dihedral style Cannot set class 2 coeffs in data file for this dihedral style.

Invalid color in dump_modify command The specified color name was not in the list of recognized colors. See the dump_modify doc page.

Invalid color map min/max values The min/max values are not consistent with either each other or with values in the color map.

Invalid command-line argument One or more command-line arguments is invalid. Check the syntax of the command you are using to launch LAMMPS.

Invalid compute ID in variable formula The compute is not recognized.

Invalid create_atoms rotation vector for 2d model The rotation vector can only have a z component.

Invalid custom OpenCL parameter string. There are not enough or too many parameters in the custom string for package GPU.

Invalid cutoff in comm_modify command Specified cutoff must be >= 0.0.

Invalid cutoffs in pair_write command Inner cutoff must be larger than 0.0 and less than outer cutoff.

Invalid d1 or d2 value for pair colloid coeff Neither d1 or d2 can be < 0.

Invalid data file section: Angle Coeffs Atom style does not allow angles.

Invalid data file section: AngleAngle Coeffs Atom style does not allow impropers.

Invalid data file section: AngleAngleTorsion Coeffs Atom style does not allow dihedrals.

Invalid data file section: AngleTorsion Coeffs Atom style does not allow dihedrals.

Invalid data file section: Angles Atom style does not allow angles.

Invalid data file section: Bodies Atom style does not allow bodies.

Invalid data file section: Bond Coeffs Atom style does not allow bonds.

Invalid data file section: BondAngle Coeffs Atom style does not allow angles.

Invalid data file section: BondBond Coeffs Atom style does not allow angles.

Invalid data file section: BondBond13 Coeffs Atom style does not allow dihedrals.

Invalid data file section: Bonds Atom style does not allow bonds.

Invalid data file section: Dihedral Coeffs Atom style does not allow dihedrals.

Invalid data file section: Dihedrals Atom style does not allow dihedrals.

Invalid data file section: Ellipsoids Atom style does not allow ellipsoids.

Invalid data file section: EndBondTorsion Coeffs Atom style does not allow dihedrals.

Invalid data file section: Improper Coeffs Atom style does not allow impropers.

Invalid data file section: Impropers Atom style does not allow impropers.

Invalid data file section: Lines Atom style does not allow lines.

Invalid data file section: MiddleBondTorsion Coeffs Atom style does not allow dihedrals.

Invalid data file section: Triangles Atom style does not allow triangles.

Invalid delta_conf in tad command The value must be between 0 and 1 inclusive.

Invalid density in Atoms section of data file Density value cannot be <= 0.0.

Invalid density in set command Density must be > 0.0.

Invalid diameter in set command Self-explanatory.

Invalid dihedral count in molecule file Self-explanatory.

Invalid dihedral type in Dihedrals section of data file Dihedral type must be positive integer and within range of specified dihedral types.

Invalid dihedral type in dihedrals section of molecule file Self-explanatory.

Invalid dipole length in set command Self-explanatory.

Invalid displace_atoms rotate axis for 2d Axis must be in z direction.

Invalid dump dcd filename Filenames used with the dump dcd style cannot be binary or compressed or cause multiple files to be written.

Invalid dump frequency Dump frequency must be 1 or greater.

Invalid dump image element name The specified element name was not in the standard list of elements. See the dump_modify doc page.

Invalid dump image filename The file produced by dump image cannot be binary and must be for a single processor.

Invalid dump image persp value Persp value must be >= 0.0.

Invalid dump image theta value Theta must be between 0.0 and 180.0 inclusive.

Invalid dump image zoom value Zoom value must be > 0.0.

Invalid dump movie filename The file produced by dump movie cannot be binary or compressed and must be a single file for a single processor.

Invalid dump xtc filename Filenames used with the dump xtc style cannot be binary or compressed or cause multiple files to be written.

Invalid dump xyz filename Filenames used with the dump xyz style cannot be binary or cause files to be written by each processor.

Invalid dump_modify threshold operator Operator keyword used for threshold specification in not recognized.

Invalid entry in -reorder file Self-explanatory.

Invalid fix ID in variable formula The fix is not recognized.

Invalid fix ave/time off column Self-explanatory.

Invalid fix box/relax command for a 2d simulation Fix box/relax styles involving the z dimension cannot be used in a 2d simulation.

Invalid fix box/relax command pressure settings If multiple dimensions are coupled, those dimensions must be specified.

Invalid fix box/relax pressure settings Settings for coupled dimensions must be the same.

Invalid fix nvt/npt/nph command for a 2d simulation Cannot control z dimension in a 2d model.

Invalid fix nvt/npt/nph command pressure settings If multiple dimensions are coupled, those dimensions must be specified.

Invalid fix nvt/npt/nph pressure settings Settings for coupled dimensions must be the same.

Invalid fix press/berendsen for a 2d simulation The z component of pressure cannot be controlled for a 2d model.

Invalid fix press/berendsen pressure settings Settings for coupled dimensions must be the same.

Invalid fix qeq parameter file Element index > number of atom types.

Invalid fix rigid npt/nph command for a 2d simulation Cannot control z dimension in a 2d model.

Invalid fix rigid npt/nph command pressure settings If multiple dimensions are coupled, those dimensions must be specified.

Invalid fix rigid/small npt/nph command for a 2d simulation Cannot control z dimension in a 2d model.

Invalid fix rigid/small npt/nph command pressure settings If multiple dimensions are coupled, those dimensions must be specified.

Invalid flag in force field section of restart file Unrecognized entry in restart file.

Invalid flag in header section of restart file Unrecognized entry in restart file.

Invalid flag in peratom section of restart file The format of this section of the file is not correct.

Invalid flag in type arrays section of restart file Unrecognized entry in restart file.

Invalid frequency in temper command Nevery must be > 0.

Invalid group ID in neigh_modify command A group ID used in the neigh_modify command does not exist.

Invalid group function in variable formula Group function is not recognized.

Invalid group in comm_modify command Self-explanatory.

Invalid image up vector Up vector cannot be (0,0,0).

Invalid immediate variable Syntax of immediate value is incorrect.

Invalid improper count in molecule file Self-explanatory.

Invalid improper type in Impropers section of data file Improper type must be positive integer and within range of specified improper types.

Invalid improper type in impropers section of molecule file Self-explanatory.

Invalid index for non-body particles in compute body/local command Only indices 1,2,3 can be used for non-body particles.

Invalid index in compute body/local command Self-explanatory.

Invalid is_active() function in variable formula Self-explanatory.

Invalid is_available() function in variable formula Self-explanatory.

Invalid is_defined() function in variable formula Self-explanatory.

Invalid keyword in angle table parameters Self-explanatory.

Invalid keyword in bond table parameters Self-explanatory.

Invalid keyword in compute angle/local command Self-explanatory.

Invalid keyword in compute bond/local command Self-explanatory.

Invalid keyword in compute dihedral/local command Self-explanatory.

Invalid keyword in compute improper/local command Self-explanatory.

Invalid keyword in compute pair/local command Self-explanatory.

Invalid keyword in compute property/atom command Self-explanatory.

Invalid keyword in compute property/chunk command Self-explanatory.

Invalid keyword in compute property/local command Self-explanatory.

Invalid keyword in dump cfg command Self-explanatory.

Invalid keyword in pair table parameters Keyword used in list of table parameters is not recognized.

Invalid length in set command Self-explanatory.

Invalid mass in set command Self-explanatory.

Invalid mass line in data file Self-explanatory.

Invalid mass value Self-explanatory.

Invalid math function in variable formula Self-explanatory.

Invalid math/group/special function in variable formula Self-explanatory.

Invalid option in lattice command for non-custom style Certain lattice keywords are not supported unless the lattice style is "custom".

Invalid order of forces within respa levels For respa, ordering of force computations within respa levels must obey certain rules. E.g. bonds cannot be compute less frequently than angles, pairwise forces cannot be computed less frequently than kspace, etc.

Invalid pair table cutoff Cutoffs in pair_coeff command are not valid with read-in pair table.

Invalid pair table length Length of read-in pair table is invalid

Invalid param file for fix qeq/shielded Invalid value of gamma.

Invalid param file for fix qeq/slater Zeta value is 0.0.

Invalid partitions in processors part command Valid partitions are numbered 1 to N and the sender and receiver cannot be the same partition.

Invalid python command Self-explanatory. Check the input script syntax and compare to the documentation for the command. You can use -echo screen as a command-line option when running LAMMPS to see the offending line.

Invalid radius in Atoms section of data file Radius must be >= 0.0.

Invalid random number seed in fix ttm command Random number seed must be > 0.

Invalid random number seed in set command Random number seed must be > 0.

Invalid replace values in compute reduce Self-explanatory.

Invalid rigid body ID in fix rigid file The ID does not match the number of an existing ID of rigid bodies that are defined by the fix rigid command.

Invalid rigid body ID in fix rigid/small file The ID does not match the number of an existing ID of rigid bodies that are defined by the fix rigid/small command.

Invalid run command N value The number of timesteps must fit in a 32-bit integer. If you want to run for more steps than this, perform multiple shorter runs.

Invalid run command start/stop value Self-explanatory.

Invalid run command upto value Self-explanatory.

Invalid seed for Marsaglia random # generator The initial seed for this random number generator must be a positive integer less than or equal to 900 million.

Invalid seed for Park random # generator The initial seed for this random number generator must be a positive integer.

Invalid shake angle type in molecule file Self-explanatory.

Invalid shake atom in molecule file Self-explanatory.

Invalid shake bond type in molecule file Self-explanatory.

Invalid shake flag in molecule file Self-explanatory.

Invalid shape in Ellipsoids section of data file Self-explanatory.

Invalid shape in Triangles section of data file Two or more of the triangle corners are duplicate points.

Invalid shape in set command Self-explanatory.

Invalid shear direction for fix wall/gran Self-explanatory.

Invalid special atom index in molecule file Self-explanatory.

Invalid special function in variable formula Self-explanatory.

Invalid style in pair_write command Self-explanatory. Check the input script.

Invalid syntax in variable formula Self-explanatory.

Invalid t_event in prd command Self-explanatory.

Invalid t_event in tad command The value must be greater than 0.

Invalid template atom in Atoms section of data file The atom indices must be between 1 to N, where N is the number of atoms in the template molecule the atom belongs to.

Invalid template index in Atoms section of data file The template indices must be between 1 to N, where N is the number of molecules in the template.

Invalid thermo keyword in variable formula The keyword is not recognized.

Invalid threads_per_atom specified. For 3-body potentials on the GPU, the threads_per_atom setting cannot be greater than 4 for NVIDIA GPUs.

Invalid timestep reset for fix ave/atom Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

Invalid timestep reset for fix ave/chunk Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

Invalid timestep reset for fix ave/correlate Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

Invalid timestep reset for fix ave/histo Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

Invalid timestep reset for fix ave/spatial Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

Invalid timestep reset for fix ave/time Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

Invalid tmax in tad command The value must be greater than 0.0.

Invalid type for mass set Mass command must set a type from 1-N where N is the number of atom types.

Invalid use of library file() function This function is called through the library interface. This error should not occur. Contact the developers if it does.

Invalid value in set command The value specified for the setting is invalid, likely because it is too small or too large.

Invalid variable evaluation in variable formula A variable used in a formula could not be evaluated.

Invalid variable in next command Self-explanatory.

Invalid variable name Variable name used in an input script line is invalid.

Invalid variable name in variable formula Variable name is not recognized.

Invalid variable style in special function next Only file-style or atomfile-style variables can be used with next().

Invalid variable style with next command Variable styles *equal* and *world* cannot be used in a next command.

Invalid volume in set command Volume must be > 0.0.

Invalid wiggle direction for fix wall/gran Self-explanatory.

Invoked angle equil angle on angle style none Self-explanatory.

Invoked angle single on angle style none Self-explanatory.

Invoked bond equil distance on bond style none Self-explanatory.

Invoked bond single on bond style none Self-explanatory.

Invoked pair single on pair style none A command (e.g. a dump) attempted to invoke the single() function on a pair style none, which is illegal. You are probably attempting to compute per-atom quantities with an undefined pair style.

Invoking coulombic in pair style lj/coul requires atom attribute q The atom style defined does not have this attribute.

Invoking coulombic in pair style lj/long/dipole/long requires atom attribute q The atom style defined does not have these attributes.

KIM Simulator Model has no Model definition There is no model definition (key: model-defn) in the KIM Simulator Model. Please contact the OpenKIM database maintainers to verify and potentially correct this.

KOKKOS package does not yet support comm_style tiled Self-explanatory.

KOKKOS package requires a kokkos enabled atom_style Self-explanatory.

KSpace accuracy must be > 0 The kspace accuracy designated in the input must be greater than zero.

KSpace accuracy too large to estimate G vector Reduce the accuracy request or specify gewald explicitly via the kspace_modify command.

KSpace accuracy too low Requested accuracy must be less than 1.0.

KSpace solver requires a pair style No pair style is defined.

KSpace style does not yet support triclinic geometries The specified kspace style does not allow for non-orthogonal simulation boxes.

KSpace style has not yet been set Cannot use kspace_modify command until a kspace style is set.

KSpace style is incompatible with Pair style Setting a kspace style requires that a pair style with matching long-range Coulombic or dispersion components be used.

Keyword %s in MEAM parameter file not recognized Self-explanatory.

Kokkos has been compiled for CUDA but no GPUs are requested One or more GPUs must be used when Kokkos is compiled for CUDA.

Kspace_modify mesh parameter must be all zero or all positive Valid kspace mesh parameters are >0. The code will try to auto-detect suitable values when all three mesh sizes are set to zero (the default).

Kspace_modify mesh/disp parameter must be all zero or all positive Valid kspace mesh/disp parameters are >0. The code will try to auto-detect suitable values when all three mesh sizes are set to zero **and** the required accuracy via *force/disp/real* as well as *force/disp/kspace* is set.

Kspace style does not support compute group/group Self-explanatory.

Kspace style pppm/disp/tip4p requires newton on Self-explanatory.

Kspace style pppm/tip4p requires newton on Self-explanatory.

Kspace style requires atom attribute q The atom style defined does not have these attributes.

Kspace_modify eigtol must be smaller than one Self-explanatory.

LAMMPS is not built with Python embedded This is done by including the PYTHON package before LAMMPS is built. This is required to use python-style variables.

LAMMPS unit_style lj not supported by KIM models Self-explanatory. Check the input script or data file.

LJ6 off not supported in pair_style buck/long/coul/long Self-explanatory.

Label wasn't found in input script Self-explanatory.

Lattice orient vectors are not orthogonal The three specified lattice orientation vectors must be mutually orthogonal.

Lattice orient vectors are not right-handed The three specified lattice orientation vectors must create a right-handed coordinate system such that a1 cross a2 = a3.

Lattice primitive vectors are collinear The specified lattice primitive vectors do not for a unit cell with non-zero volume.

Lattice settings are not compatible with 2d simulation One or more of the specified lattice vectors has a non-zero z component.

Lattice spacings are invalid Each x,y,z spacing must be > 0.

Lattice style incompatible with simulation dimension 2d simulation can use sq, sq2, or hex lattice. 3d simulation can use sc, bcc, or fcc lattice.

Log of zero/negative value in variable formula Self-explanatory.

Lost atoms via balance: original %ld current %ld This should not occur. Report the problem to the developers.

Lost atoms: original %ld current %ld Lost atoms are checked for each time thermo output is done. See the thermo_modify lost command for options. Lost atoms usually indicate bad dynamics, e.g. atoms have been blown far out of the simulation box, or moved further than one processor's sub-domain away before reneighboring.

MEAM library error %d A call to the MEAM Fortran library returned an error.

MPI_LMP_BIGINT and bigint in lmptype.h are not compatible The size of the MPI datatype does not match the size of a bigint.

MPI_LMP_TAGINT and tagint in lmptype.h are not compatible The size of the MPI datatype does not match the size of a tagint.

MSM can only currently be used with comm_style brick This is a current restriction in LAMMPS.

MSM grid is too large The global MSM grid is larger than OFFSET in one or more dimensions. OFFSET is currently set to 16384. You likely need to decrease the requested accuracy.

MSM order must be 4, 6, 8, or 10 This is a limitation of the MSM implementation in LAMMPS: the MSM order can only be 4, 6, 8, or 10.

Mass command before simulation box is defined The mass command cannot be used before a read_data, read_restart, or create_box command.

Matrix factorization to split dispersion coefficients failed This should not normally happen. Contact the developers.

Min_style command before simulation box is defined The min_style command cannot be used before a read_data, read_restart, or create_box command.

Minimization could not find thermo_pe compute This compute is created by the thermo command. It must have been explicitly deleted by a uncompute command.

Minimize command before simulation box is defined The minimize command cannot be used before a read_data, read_restart, or create_box command.

Mismatched brackets in variable Self-explanatory.

Mismatched compute in variable formula A compute is referenced incorrectly or a compute that produces per-atom values is used in an equal-style variable formula.

Mismatched fix in variable formula A fix is referenced incorrectly or a fix that produces per-atom values is used in an equal-style variable formula.

Mismatched variable in variable formula A variable is referenced incorrectly or an atom-style variable that produces per-atom values is used in an equal-style variable formula.

Modulo 0 in variable formula Self-explanatory.

Molecule IDs too large for compute chunk/atom The IDs must not be larger than can be stored in a 32-bit integer since chunk IDs are 32-bit integers.

Molecule auto special bond generation overflow Counts exceed maxspecial setting for other atoms in system.

Molecule file has angles but no nangles setting Self-explanatory.

Molecule file has body params but no setting for them Self-explanatory.

Molecule file has bonds but no nbonds setting Self-explanatory.

Molecule file has dihedrals but no ndihedrals setting Self-explanatory.

Molecule file has impropers but no nimpropers setting Self-explanatory.

Molecule file has no Body Doubles section Self-explanatory.

Molecule file has no Body Integers section Self-explanatory.

Molecule file has special flags but no bonds Self-explanatory.

Molecule file needs both Special Bond sections Self-explanatory.

Molecule file requires atom style body Self-explanatory.

Molecule file shake flags not before shake atoms The order of the two sections is important.

Molecule file shake flags not before shake bonds The order of the two sections is important.

Molecule file shake info is incomplete All 3 SHAKE sections are needed.

Molecule file special list does not match special count The number of values in an atom's special list does not match count.

Molecule file z center-of-mass must be 0.0 for 2d Self-explanatory.

Molecule file z coord must be 0.0 for 2d Self-explanatory.

Molecule natoms must be 1 for body particle Self-explanatory.

Molecule sizescale must be 1.0 for body particle Self-explanatory.

Molecule template ID for atom_style template does not exist Self-explanatory.

Molecule template ID for create_atoms does not exist Self-explanatory.

Molecule template ID for fix deposit does not exist Self-explanatory.

Molecule template ID for fix gcmc does not exist Self-explanatory.

Molecule template ID for fix pour does not exist Self-explanatory.

Molecule template ID for fix rigid/small does not exist Self-explanatory.

Molecule template ID for fix shake does not exist Self-explanatory.

Molecule template ID must be alphanumeric or underscore characters Self-explanatory.

Molecule topology/atom exceeds system topology/atom The number of bonds, angles, etc per-atom in the molecule exceeds the system setting. See the create_box command for how to specify these values.

Molecule topology type exceeds system topology type The number of bond, angle, etc types in the molecule exceeds the system setting. See the create_box command for how to specify these values.

More than one fix deform Only one fix deform can be defined at a time.

More than one fix freeze Only one of these fixes can be defined, since the granular pair potentials access it.

More than one fix shake Only one fix shake can be defined.

Mu not allowed when not using semi-grand in fix atom/swap command Self-explanatory.

Must define angle_style before Angle Coeffs Must use an angle_style command before reading a data file that defines Angle Coeffs.

Must define angle_style before BondAngle Coeffs Must use an angle_style command before reading a data file that defines Angle Coeffs.

Must define angle_style before BondBond Coeffs Must use an angle_style command before reading a data file that defines Angle Coeffs.

Must define bond_style before Bond Coeffs Must use a bond_style command before reading a data file that defines Bond Coeffs.

Must define dihedral_style before AngleAngleTorsion Coeffs Must use a dihedral_style command before reading a data file that defines AngleAngleTorsion Coeffs.

Must define dihedral_style before AngleTorsion Coeffs Must use a dihedral_style command before reading a data file that defines AngleTorsion Coeffs.

Must define dihedral_style before BondBond13 Coeffs Must use a dihedral_style command before reading a data file that defines BondBond13 Coeffs.

Must define dihedral_style before Dihedral Coeffs Must use a dihedral_style command before reading a data file that defines Dihedral Coeffs.

Must define dihedral_style before EndBondTorsion Coeffs Must use a dihedral_style command before reading a data file that defines EndBondTorsion Coeffs.

Must define dihedral_style before MiddleBondTorsion Coeffs Must use a dihedral_style command before reading a data file that defines MiddleBondTorsion Coeffs.

Must define improper_style before AngleAngle Coeffs Must use an improper_style command before reading a data file that defines AngleAngle Coeffs.

Must define improper_style before Improper Coeffs Must use an improper_style command before reading a data file that defines Improper Coeffs.

Must define pair_style before Pair Coeffs Must use a pair_style command before reading a data file that defines Pair Coeffs.

Must define pair_style before PairIJ Coeffs Must use a pair_style command before reading a data file that defines PairIJ Coeffs.

Must have more than one processor partition to temper Cannot use the temper command with only one processor partition. Use the -partition command-line option.

Must read Atoms before Angles The Atoms section of a data file must come before an Angles section.

Must read Atoms before Bodies The Atoms section of a data file must come before a Bodies section.

Must read Atoms before Bonds The Atoms section of a data file must come before a Bonds section.

Must read Atoms before Dihedrals The Atoms section of a data file must come before a Dihedrals section.

Must read Atoms before Ellipsoids The Atoms section of a data file must come before a Ellipsoids section.

Must read Atoms before Impropers The Atoms section of a data file must come before an Impropers section.

Must read Atoms before Lines The Atoms section of a data file must come before a Lines section.

Must read Atoms before Triangles The Atoms section of a data file must come before a Triangles section.

Must read Atoms before Velocities The Atoms section of a data file must come before a Velocities section.

Must re-specify non-restarted pair style (xxx) after read_restart For pair styles, that do not store their settings in a restart file, it must be defined with a new 'pair_style' command after read_restart.

Must set both respa inner and outer Cannot use just the inner or outer option with respa without using the other.

Must set number of threads via package omp command Because you are using the USER-OMP package, set the number of threads via its settings, not by the pair_style snap nthreads setting.

Must shrink-wrap piston boundary The boundary style of the face where the piston is applied must be of type s (shrink-wrapped).

Must specify a region in fix deposit The region keyword must be specified with this fix.

Must specify a region in fix pour Self-explanatory.

Must specify at least 2 types in fix atom/swap command Self-explanatory.

Must use 'kim_style init' command before simulation box is defined Self-explanatory.

Must use 'kim_style define' command after simulation box is defined Self-explanatory.

Must use 'kim_style init' command before 'kim_style define' Self-explanatory.

Must use 'kspace_modify pressure/scalar no' for rRESPA with kspace_style MSM The kspace scalar pressure option cannot (yet) be used with rRESPA.

Must use 'kspace_modify pressure/scalar no' for tensor components with kspace_style msm Otherwise MSM will compute only a scalar pressure. See the kspace_modify command for details on this setting.

Must use 'kspace_modify pressure/scalar no' to obtain per-atom virial with kspace_style MSM The kspace scalar pressure option cannot be used to obtain per-atom virial.

Must use 'kspace_modify pressure/scalar no' with GPU MSM Pair styles The kspace scalar pressure option is not (yet) compatible with GPU MSM Pair styles.

Must use 'kspace_modify pressure/scalar no' with kspace_style msm/cg The kspace scalar pressure option is not compatible with kspace_style msm/cg.

Must use -in switch with multiple partitions A multi-partition simulation cannot read the input script from stdin. The -in command-line option must be used to specify a file.

Must use Kokkos half/thread or full neighbor list with threads or GPUs Using Kokkos half-neighbor lists with threading is not allowed.

Must use a block or cylinder region with fix pour Self-explanatory.

Must use a block region with fix pour for 2d simulations Self-explanatory.

Must use a bond style with TIP4P potential TIP4P potentials assume bond lengths in water are constrained by a fix shake command.

Must use a molecular atom style with fix poems molecule Self-explanatory.

Must use a z-axis cylinder region with fix pour Self-explanatory.

Must use an angle style with TIP4P potential TIP4P potentials assume angles in water are constrained by a fix shake command.

Must use atom map style array with Kokkos See the atom_modify map command.

Must use atom style with molecule IDs with fix bond/swap Self-explanatory.

Must use pair_style comb or comb3 with fix qeq/comb Self-explanatory.

Must use variable energy with fix addforce Must define an energy variable when applying a dynamic force during minimization.

Must use variable energy with fix efield You must define an energy when performing a minimization with a variable E-field.

NEB command before simulation box is defined Self-explanatory.

NEB requires damped dynamics minimizer Use a different minimization style.

NEB requires use of fix neb Self-explanatory.

NL ramp in wall/piston only implemented in zlo for now The ramp keyword can only be used for piston applied to face zlo.

Need nswaptypes mu values in fix atom/swap command Self-explanatory.

Needed bonus data not in data file Some atom styles require bonus data. See the read_data doc page for details.

Needed molecular topology not in data file The header of the data file indicated bonds, angles, etc would be included, but they are not present.

Neigh_modify exclude molecule requires atom attribute molecule Self-explanatory.

Neigh_modify include group != atom_modify first group Self-explanatory.

Neighbor delay must be 0 or multiple of every setting The delay and every parameters set via the neigh_modify command are inconsistent. If the delay setting is non-zero, then it must be a multiple of the every setting.

Neighbor include group not allowed with ghost neighbors This is a current restriction within LAMMPS.

Neighbor list overflow, boost neigh_modify one There are too many neighbors of a single atom. Use the neigh_modify command to increase the max number of neighbors allowed for one atom. You may also want to boost the page size.

Neighbor multi not yet enabled for ghost neighbors This is a current restriction within LAMMPS.

Neighbor multi not yet enabled for granular Self-explanatory.

Neighbor multi not yet enabled for rRESPA Self-explanatory.

Neighbor page size must be >= 10x the one atom setting This is required to prevent wasting too much memory.

New atom IDs exceed maximum allowed ID See the setting for tagint in the src/lmptype.h file.

New bond exceeded bonds per atom in create_bonds See the read_data command for info on using the "extra/bond/per/atom" keyword to allow for additional bonds to be formed

New bond exceeded bonds per atom in fix bond/create See the read_data command for info on using the "extra/bond/per/atom" keyword to allow for additional bonds to be formed

New bond exceeded special list size in fix bond/create See the "read_data extra/special/per/atom" command (or the "create_box extra/special/per/atom" command) for info on how to leave space in the special bonds list to allow for additional bonds to be formed.

Newton bond change after simulation box is defined The newton command cannot be used to change the newton bond value after a read_data, read_restart, or create_box command.

Next command must list all universe and uloop variables This is to insure they stay in sync.

No Kspace style defined for compute group/group Self-explanatory.

No OpenMP support compiled in An OpenMP flag is set, but LAMMPS was not built with OpenMP support.

No angle style is defined for compute angle/local Self-explanatory.

No angles allowed with this atom style Self-explanatory.

No atoms in data file The header of the data file indicated that atoms would be included, but they are not present.

No basis atoms in lattice Basis atoms must be defined for lattice style user.

No bodies allowed with this atom style Self-explanatory. Check data file.

No bond style is defined for compute bond/local Self-explanatory.

No bonds allowed with this atom style Self-explanatory.

No box information in dump. You have to use 'box no' Self-explanatory.

No count or invalid atom count in molecule file The number of atoms must be specified.

No dihedral style is defined for compute dihedral/local Self-explanatory.

No dihedrals allowed with this atom style Self-explanatory.

No dump custom arguments specified The dump custom command requires that atom quantities be specified to output to dump file.

No dump local arguments specified Self-explanatory.

No ellipsoids allowed with this atom style Self-explanatory. Check data file.

No fix gravity defined for fix pour Gravity is required to use fix pour.

No improper style is defined for compute improper/local Self-explanatory.

No impropers allowed with this atom style Self-explanatory.

No input values for fix ave/spatial Self-explanatory.

No lines allowed with this atom style Self-explanatory. Check data file.

No matching element in ADP potential file The ADP potential file does not contain elements that match the requested elements.

No matching element in EAM potential file The EAM potential file does not contain elements that match the requested elements.

No molecule topology allowed with atom style template The data file cannot specify the number of bonds, angles, etc, because this info if inferred from the molecule templates.

No overlap of box and region for create_atoms Self-explanatory.

No pair coul/streitz for fix qeq/slater These commands must be used together.

No pair hbond/dreiding coefficients set Self-explanatory.

No pair style defined for compute group/group Cannot calculate group interactions without a pair style defined.

No pair style is defined for compute pair/local Self-explanatory.

No pair style is defined for compute property/local Self-explanatory.

No rigid bodies defined The fix specification did not end up defining any rigid bodies.

No triangles allowed with this atom style Self-explanatory. Check data file.

No values in fix ave/chunk command Self-explanatory.

No values in fix ave/time command Self-explanatory.

Non digit character between brackets in variable Self-explanatory.

Non integer # of swaps in temper command Swap frequency in temper command must evenly divide the total # of timesteps.

Non-numeric box dimensions - simulation unstable The box size has apparently blown up.

Non-zero atom IDs with atom_modify id = no Self-explanatory.

Non-zero read_data shift z value for 2d simulation Self-explanatory.

Nprocs not a multiple of N for -reorder Self-explanatory.

Number of core atoms != number of shell atoms There must be a one-to-one pairing of core and shell atoms.

Numeric index is out of bounds A command with an argument that specifies an integer or range of integers is using a value that is less than 1 or greater than the maximum allowed limit.

One or more Atom IDs is negative Atom IDs must be positive integers.

One or more atom IDs is too big The limit on atom IDs is set by the SMALLBIG, BIGBIG, SMALLSMALL setting in your LAMMPS build. See the *Build settings* doc page for more info.

One or more atom IDs is zero Either all atoms IDs must be zero or none of them.

One or more atoms belong to multiple rigid bodies Two or more rigid bodies defined by the fix rigid command cannot contain the same atom.

One or more rigid bodies are a single particle Self-explanatory.

One or zero atoms in rigid body Any rigid body defined by the fix rigid command must contain 2 or more atoms.

Only 2 types allowed when not using semi-grand in fix atom/swap command Self-explanatory.

Only one cut-off allowed when requesting all long Self-explanatory.

Only one cutoff allowed when requesting all long Self-explanatory.

Only zhi currently implemented for fix append/atoms Self-explanatory.

Out of range atoms - cannot compute MSM One or more atoms are attempting to map their charge to a MSM grid point that is not owned by a processor. This is likely for one of two reasons, both of them bad. First, it may mean that an atom near the boundary of a processor's sub-domain has moved more than 1/2 the *neighbor skin distance* without neighbor lists being rebuilt and atoms being migrated to new processors. This also means you may be missing pairwise interactions that need to be computed. The solution is to change the re-neighboring criteria via the *neigh_modify* command. The safest settings are "delay 0 every 1 check yes". Second, it may mean that an atom has moved far outside a processor's sub-domain or even the entire simulation box. This indicates bad physics, e.g. due to highly overlapping atoms, too large a timestep, etc.

Out of range atoms - cannot compute PPPM One or more atoms are attempting to map their charge to a PPPM grid point that is not owned by a processor. This is likely for one of two reasons, both of them bad. First, it may mean that an atom near the boundary of a processor's sub-domain has moved more than 1/2 the *neighbor skin distance* without neighbor lists being rebuilt and atoms being migrated to new processors. This also means you may be missing pairwise interactions that need to be computed. The solution is to change the re-neighboring criteria via the *neigh_modify* command. The safest settings are "delay 0 every 1 check yes". Second, it may mean that an atom has moved far outside a processor's sub-domain or even the entire simulation box. This indicates bad physics, e.g. due to highly overlapping atoms, too large a timestep, etc.

Out of range atoms - cannot compute PPPMDisp One or more atoms are attempting to map their charge to a PPPM grid point that is not owned by a processor. This is likely for one of two reasons, both of them bad. First, it may mean that an atom near the boundary of a processor's sub-domain has moved more than 1/2 the *neighbor skin distance* without neighbor lists being rebuilt and atoms being migrated to new processors. This also means you may be missing pairwise interactions that need to be computed. The solution is to change the re-neighboring criteria via the *neigh_modify* command. The safest settings are "delay 0 every 1 check yes". Second, it may mean that an atom has moved far outside a processor's sub-domain or even the entire simulation box. This indicates bad physics, e.g. due to highly overlapping atoms, too large a timestep, etc.

Overflow of allocated fix vector storage This should not normally happen if the fix correctly calculated how long the vector will grow to. Contact the developers.

Overlapping large/large in pair colloid This potential is infinite when there is an overlap.

Overlapping small/large in pair colloid This potential is infinite when there is an overlap.

POEMS fix must come before NPT/NPH fix NPT/NPH fix must be defined in input script after all poems fixes, else the fix contribution to the pressure virial is incorrect.

PPPM can only currently be used with comm_style brick This is a current restriction in LAMMPS.

PPPM grid is too large The global PPPM grid is larger than OFFSET in one or more dimensions. OFFSET is currently set to 4096. You likely need to decrease the requested accuracy.

PPPM grid stencil extends beyond nearest neighbor processor This is not allowed if the kspace_modify overlap setting is no.

PPPM order < minimum allowed order The default minimum order is 2. This can be reset by the kspace_modify minorder command.

PPPM order cannot be < 2 or > than %d This is a limitation of the PPPM implementation in LAMMPS.

PPPMDisp Coulomb grid is too large The global PPPM grid is larger than OFFSET in one or more dimensions. OFFSET is currently set to 4096. You likely need to decrease the requested accuracy.

PPPMDisp Dispersion grid is too large The global PPPM grid is larger than OFFSET in one or more dimensions. OFFSET is currently set to 4096. You likely need to decrease the requested accuracy.

PPPMDisp can only currently be used with comm_style brick This is a current restriction in LAMMPS.

PPPMDisp coulomb order cannot be greater than %d This is a limitation of the PPPM implementation in LAMMPS.

PPPMDisp used but no parameters set, for further information please see the pppm/disp documentation An efficient and accurate usage of the pppm/disp requires settings via the kspace_modify command. Please see the pppm/disp documentation for further instructions.

PRD command before simulation box is defined The prd command cannot be used before a read_data, read_restart, or create_box command.

PRD nsteps must be multiple of t_event Self-explanatory.

PRD t_corr must be multiple of t_event Self-explanatory.

Package command after simulation box is defined The package command cannot be used after a read_data, read_restart, or create_box command.

Package gpu command without GPU package installed The GPU package must be installed via "make yes-gpu" before LAMMPS is built.

Package intel command without USER-INTEL package installed The USER-INTEL package must be installed via "make yes-user-intel" before LAMMPS is built.

Package kokkos command without KOKKOS package enabled The KOKKOS package must be installed via "make yes-kokkos" before LAMMPS is built, and the "-k on" must be used to enable the package.

Package omp command without USER-OMP package installed The USER-OMP package must be installed via "make yes-user-omp" before LAMMPS is built.

Pair body requires atom style body Self-explanatory.

Pair body requires body style nparticle This pair style is specific to the nparticle body style.

Pair brownian requires atom style sphere Self-explanatory.

Pair brownian requires extended particles One of the particles has radius 0.0.

Pair brownian requires monodisperse particles All particles must be the same finite size.

Pair brownian/poly requires atom style sphere Self-explanatory.

Pair brownian/poly requires extended particles One of the particles has radius 0.0.

Pair brownian/poly requires newton pair off Self-explanatory.

Pair coeff for hybrid has invalid style Style in pair coeff must have been listed in pair_style command.

Pair coul/wolf requires atom attribute q The atom style defined does not have this attribute.

Pair cutoff < Respa interior cutoff One or more pairwise cutoffs are too short to use with the specified rRESPA cutoffs.

Pair dipole/cut requires atom attributes q, mu, torque The atom style defined does not have these attributes.

Pair dipole/cut/gpu requires atom attributes q, mu, torque The atom style defined does not have this attribute.

Pair dipole/long requires atom attributes q, mu, torque The atom style defined does not have these attributes.

Pair dipole/sf/gpu requires atom attributes q, mu, torque The atom style defined does not one or more of these attributes.

Pair distance < table inner cutoff Two atoms are closer together than the pairwise table allows.

Pair distance > table outer cutoff Two atoms are further apart than the pairwise table allows.

Pair dpd requires ghost atoms store velocity Use the comm_modify vel yes command to enable this.

Pair gayberne epsilon a,b,c coeffs are not all set Each atom type involved in pair_style gayberne must have these 3 coefficients set at least once.

Pair gayberne requires atom style ellipsoid Self-explanatory.

Pair gayberne requires atoms with same type have same shape Self-explanatory.

Pair gayberne/gpu requires atom style ellipsoid Self-explanatory.

Pair gayberne/gpu requires atoms with same type have same shape Self-explanatory.

Pair granular requires atom attributes radius, rmass The atom style defined does not have these attributes.

Pair granular requires ghost atoms store velocity Use the comm_modify vel yes command to enable this.

Pair granular with shear history requires newton pair off This is a current restriction of the implementation of pair granular styles with history.

Pair hybrid single calls do not support per sub-style special bond values Self-explanatory.

Pair hybrid sub-style does not support single call You are attempting to invoke a single() call on a pair style that doesn't support it.

Pair hybrid sub-style is not used No pair_coeff command used a sub-style specified in the pair_style command.

Pair inner cutoff < Respa interior cutoff One or more pairwise cutoffs are too short to use with the specified rRESPA cutoffs.

Pair inner cutoff >= Pair outer cutoff The specified cutoffs for the pair style are inconsistent.

Pair line/lj requires atom style line Self-explanatory.

Pair lj/long/dipole/long requires atom attributes mu, torque The atom style defined does not have these attributes.

Pair lubricate requires atom style sphere Self-explanatory.

Pair lubricate requires ghost atoms store velocity Use the comm_modify vel yes command to enable this.

Pair lubricate requires monodisperse particles All particles must be the same finite size.

Pair lubricate/poly requires atom style sphere Self-explanatory.

Pair lubricate/poly requires extended particles One of the particles has radius 0.0.

Pair lubricate/poly requires ghost atoms store velocity Use the comm_modify vel yes command to enable this.

Pair lubricate/poly requires newton pair off Self-explanatory.

Pair lubricateU requires atom style sphere Self-explanatory.

Pair lubricateU requires ghost atoms store velocity Use the comm_modify vel yes command to enable this.

Pair lubricateU requires monodisperse particles All particles must be the same finite size.

Pair lubricateU/poly requires ghost atoms store velocity Use the comm_modify vel yes command to enable this.

Pair lubricateU/poly requires newton pair off Self-explanatory.

Pair peri lattice is not identical in x, y, and z The lattice defined by the lattice command must be cubic.

Pair peri requires a lattice be defined Use the lattice command for this purpose.

Pair peri requires an atom map, see atom_modify Even for atomic systems, an atom map is required to find Peridynamic bonds. Use the atom_modify command to define one.

Pair resquared epsilon a,b,c coeffs are not all set Self-explanatory.

Pair resquared epsilon and sigma coeffs are not all set Self-explanatory.

Pair resquared requires atom style ellipsoid Self-explanatory.

Pair resquared requires atoms with same type have same shape Self-explanatory.

Pair resquared/gpu requires atom style ellipsoid Self-explanatory.

Pair resquared/gpu requires atoms with same type have same shape Self-explanatory.

Pair style AIREBO requires atom IDs This is a requirement to use the AIREBO potential.

Pair style AIREBO requires newton pair on See the newton command. This is a restriction to use the AIREBO potential.

Pair style BOP requires atom IDs This is a requirement to use the BOP potential.

Pair style BOP requires newton pair on See the newton command. This is a restriction to use the BOP potential.

Pair style COMB requires atom IDs This is a requirement to use the AIREBO potential.

Pair style COMB requires atom attribute q Self-explanatory.

Pair style COMB requires newton pair on See the newton command. This is a restriction to use the COMB potential.

Pair style COMB3 requires atom IDs This is a requirement to use the COMB3 potential.

Pair style COMB3 requires atom attribute q Self-explanatory.

Pair style COMB3 requires newton pair on See the newton command. This is a restriction to use the COMB3 potential.

Pair style LCBOP requires atom IDs This is a requirement to use the LCBOP potential.

Pair style LCBOP requires newton pair on See the newton command. This is a restriction to use the Tersoff potential.

Pair style MEAM requires newton pair on See the newton command. This is a restriction to use the MEAM potential.

Pair style SNAP requires newton pair on See the newton command. This is a restriction to use the SNAP potential.

Pair style Stillinger-Weber requires atom IDs This is a requirement to use the SW potential.

Pair style Stillinger-Weber requires newton pair on See the newton command. This is a restriction to use the SW potential.

Pair style Tersoff requires atom IDs This is a requirement to use the Tersoff potential.

Pair style Tersoff requires newton pair on See the newton command. This is a restriction to use the Tersoff potential.

Pair style Vashishta requires atom IDs This is a requirement to use the Vashishta potential.

Pair style Vashishta requires newton pair on See the newton command. This is a restriction to use the Vashishta potential.

Pair style bop requires comm ghost cutoff at least 3x larger than %g Use the communicate ghost command to set this. See the pair bop doc page for more details.

Pair style born/coul/long requires atom attribute q An atom style that defines this attribute must be used.

Pair style born/coul/long/gpu requires atom attribute q The atom style defined does not have this attribute.

Pair style born/coul/wolf requires atom attribute q The atom style defined does not have this attribute.

Pair style buck/coul/cut requires atom attribute q The atom style defined does not have this attribute.

Pair style buck/coul/long requires atom attribute q The atom style defined does not have these attributes.

Pair style buck/coul/long/gpu requires atom attribute q The atom style defined does not have this attribute.

Pair style buck/long/coul/long requires atom attribute q The atom style defined does not have this attribute.

Pair style coul/cut requires atom attribute q The atom style defined does not have these attributes.

Pair style coul/cut/gpu requires atom attribute q The atom style defined does not have this attribute.

Pair style coul/debye/gpu requires atom attribute q The atom style defined does not have this attribute.

Pair style coul/dsf requires atom attribute q The atom style defined does not have this attribute.

Pair style coul/dsf/gpu requires atom attribute q The atom style defined does not have this attribute.

Pair style coul/long/gpu requires atom attribute q The atom style defined does not have these attributes.

Pair style coul/streitz requires atom attribute q Self-explanatory.

Pair style does not have extra field requested by compute pair/local The pair style does not support the pN value requested by the compute pair/local command.

Pair style does not support bond_style quartic The pair style does not have a single() function, so it can not be invoked by bond_style quartic.

Pair style does not support compute group/group The pair_style does not have a single() function, so it cannot be invoked by the compute group/group command.

Pair style does not support compute pair/local The pair style does not have a single() function, so it can not be invoked by compute pair/local.

Pair style does not support compute property/local The pair style does not have a single() function, so it can not be invoked by fix bond/swap.

Pair style does not support fix bond/swap The pair style does not have a single() function, so it can not be invoked by fix bond/swap.

Pair style does not support pair_write The pair style does not have a single() function, so it can not be invoked by pair write.

Pair style does not support rRESPA inner/middle/outer You are attempting to use rRESPA options with a pair style that does not support them.

Pair style granular with history requires atoms have IDs Atoms in the simulation do not have IDs, so history effects cannot be tracked by the granular pair potential.

Pair style hbond/dreiding requires an atom map, see atom_modify Self-explanatory.

Pair style hbond/dreiding requires atom IDs Self-explanatory.

Pair style hbond/dreiding requires molecular system Self-explanatory.

Pair style hbond/dreiding requires newton pair on See the newton command for details.

Pair style hybrid cannot have hybrid as an argument Self-explanatory.

Pair style hybrid cannot have none as an argument Self-explanatory.

Pair style is incompatible with KSpace style If a pair style with a long-range Coulombic component is selected, then a kspace style must also be used.

Pair style is incompatible with TIP4P KSpace style The pair style does not have the requires TIP4P settings.

Pair style lj/charmm/coul/charmm requires atom attribute q The atom style defined does not have these attributes.

Pair style lj/charmm/coul/long requires atom attribute q The atom style defined does not have these attributes.

Pair style lj/charmm/coul/long/gpu requires atom attribute q The atom style defined does not have this attribute.

Pair style lj/class2/coul/cut requires atom attribute q The atom style defined does not have this attribute.

Pair style lj/class2/coul/long requires atom attribute q The atom style defined does not have this attribute.

Pair style lj/class2/coul/long/gpu requires atom attribute q The atom style defined does not have this attribute.

Pair style lj/cut/coul/cut requires atom attribute q The atom style defined does not have this attribute.

Pair style lj/cut/coul/cut/gpu requires atom attribute q The atom style defined does not have this attribute.

Pair style lj/cut/coul/debye/gpu requires atom attribute q The atom style defined does not have this attribute.

Pair style lj/cut/coul/dsf requires atom attribute q The atom style defined does not have these attributes.

Pair style lj/cut/coul/dsf/gpu requires atom attribute q The atom style defined does not have this attribute.

Pair style lj/cut/coul/long requires atom attribute q The atom style defined does not have this attribute.

Pair style lj/cut/coul/long/gpu requires atom attribute q The atom style defined does not have this attribute.

Pair style lj/cut/tip4p/cut requires atom IDs This is a requirement to use this potential.

Pair style lj/cut/tip4p/cut requires atom attribute q The atom style defined does not have this attribute.

Pair style lj/cut/tip4p/cut requires newton pair on See the newton command. This is a restriction to use this potential.

Pair style lj/cut/tip4p/long requires atom IDs There are no atom IDs defined in the system and the TIP4P potential requires them to find O,H atoms with a water molecule.

Pair style lj/cut/tip4p/long requires atom attribute q The atom style defined does not have these attributes.

Pair style lj/cut/tip4p/long requires newton pair on This is because the computation of constraint forces within a water molecule adds forces to atoms owned by other processors.

Pair style lj/gromacs/coul/gromacs requires atom attribute q An atom_style with this attribute is needed.

Pair style lj/long/dipole/long does not currently support respa This feature is not yet supported.

Pair style lj/long/tip4p/long requires atom IDs There are no atom IDs defined in the system and the TIP4P potential requires them to find O,H atoms with a water molecule.

Pair style lj/long/tip4p/long requires atom attribute q The atom style defined does not have these attributes.

Pair style lj/long/tip4p/long requires newton pair on This is because the computation of constraint forces within a water molecule adds forces to atoms owned by other processors.

Pair style lj/sdk/coul/long/gpu requires atom attribute q The atom style defined does not have this attribute.

Pair style nb3b/harmonic requires atom IDs This is a requirement to use this potential.

Pair style nb3b/harmonic requires newton pair on See the newton command. This is a restriction to use this potential.

Pair style nm/cut/coul/cut requires atom attribute q The atom style defined does not have this attribute.

Pair style nm/cut/coul/long requires atom attribute q The atom style defined does not have this attribute.

Pair style peri requires atom style peri Self-explanatory.

Pair style polymorphic requires atom IDs This is a requirement to use the polymorphic potential.

Pair style polymorphic requires newton pair on See the newton command. This is a restriction to use the polymorphic potential.

Pair style reax requires atom IDs This is a requirement to use the ReaxFF potential.

Pair style reax requires atom attribute q The atom style defined does not have this attribute.

Pair style reax requires newton pair on This is a requirement to use the ReaxFF potential.

Pair style requires a KSpace style No kspace style is defined.

Pair style requires use of kspace_style ewald/disp Self-explanatory.

Pair style sw/gpu requires atom IDs This is a requirement to use this potential.

Pair style sw/gpu requires newton pair off See the newton command. This is a restriction to use this potential.

Pair style vashishta/gpu requires atom IDs This is a requirement to use this potential.

Pair style vashishta/gpu requires newton pair off See the newton command. This is a restriction to use this potential.

Pair style tersoff/gpu requires atom IDs This is a requirement to use the tersoff/gpu potential.

Pair style tersoff/gpu requires newton pair off See the newton command. This is a restriction to use this pair style.

Pair style tip4p/cut requires atom IDs This is a requirement to use this potential.

Pair style tip4p/cut requires atom attribute q The atom style defined does not have this attribute.

Pair style tip4p/cut requires newton pair on See the newton command. This is a restriction to use this potential.

Pair style tip4p/long requires atom IDs There are no atom IDs defined in the system and the TIP4P potential requires them to find O,H atoms with a water molecule.

Pair style tip4p/long requires atom attribute q The atom style defined does not have these attributes.

Pair style tip4p/long requires newton pair on This is because the computation of constraint forces within a water molecule adds forces to atoms owned by other processors.

Pair table cutoffs must all be equal to use with KSpace When using pair style table with a long-range KSpace solver, the cutoffs for all atom type pairs must all be the same, since the long-range solver starts at that cutoff.

Pair table parameters did not set N List of pair table parameters must include N setting.

Pair tersoff/zbl requires metal or real units This is a current restriction of this pair potential.

Pair tersoff/zbl/kk requires metal or real units This is a current restriction of this pair potential.

Pair tri/lj requires atom style tri Self-explanatory.

Pair yukawa/colloid requires atom style sphere Self-explanatory.

Pair yukawa/colloid requires atoms with same type have same radius Self-explanatory.

Pair yukawa/colloid/gpu requires atom style sphere Self-explanatory.

PairKIM only works with 3D problems This is a current limitation.

Pair_coeff command before pair_style is defined Self-explanatory.

Pair_coeff command before simulation box is defined The pair_coeff command cannot be used before a read_data, read_restart, or create_box command.

Pair_modify command before pair_style is defined Self-explanatory.

Pair_modify special setting for pair hybrid incompatible with global special_bonds setting Cannot override a setting of 0.0 or 1.0 or change a setting between 0.0 and 1.0.

Pair_write command before pair_style is defined Self-explanatory.

Particle on or inside fix wall surface Particles must be "exterior" to the wall in order for energy/force to be calculated.

Particle outside surface of region used in fix wall/region Particles must be inside the region for energy/force to be calculated. A particle outside the region generates an error.

Per-atom compute in equal-style variable formula Equal-style variables cannot use per-atom quantities.

Per-atom energy was not tallied on needed timestep You are using a thermo keyword that requires potentials to have tallied energy, but they didn't on this timestep. See the variable doc page for ideas on how to make this work.

Per-atom fix in equal-style variable formula Equal-style variables cannot use per-atom quantities.

Per-atom virial was not tallied on needed timestep You are using a thermo keyword that requires potentials to have tallied the virial, but they didn't on this timestep. See the variable doc page for ideas on how to make this work.

Per-processor system is too big The number of owned atoms plus ghost atoms on a single processor must fit in 32-bit integer.

Potential energy ID for fix neb does not exist Self-explanatory.

Potential energy ID for fix nvt/nph/npt does not exist A compute for potential energy must be defined.

Potential file has duplicate entry The potential file has more than one entry for the same element.

Potential file is missing an entry The potential file does not have a needed entry.

Power by 0 in variable formula Self-explanatory.

Pressure ID for fix box/relax does not exist The compute ID needed to compute pressure for the fix does not exist.

Pressure ID for fix modify does not exist Self-explanatory.

Pressure ID for fix npt/nph does not exist Self-explanatory.

Pressure ID for fix press/berendsen does not exist The compute ID needed to compute pressure for the fix does not exist.

Pressure ID for fix rigid npt/nph does not exist Self-explanatory.

Pressure ID for thermo does not exist The compute ID needed to compute pressure for thermodynamics does not exist.

Pressure control can not be used with fix nvt Self-explanatory.

Pressure control can not be used with fix nvt/asphere Self-explanatory.

Pressure control can not be used with fix nvt/body Self-explanatory.

Pressure control can not be used with fix nvt/sllod Self-explanatory.

Pressure control can not be used with fix nvt/sphere Self-explanatory.

Pressure control must be used with fix nph Self-explanatory.

Pressure control must be used with fix nph/asphere Self-explanatory.

Pressure control must be used with fix nph/body Self-explanatory.

Pressure control must be used with fix nph/small Self-explanatory.

Pressure control must be used with fix nph/sphere Self-explanatory.

Pressure control must be used with fix nphug A pressure control keyword (iso, aniso, tri, x, y, or z) must be provided.

Pressure control must be used with fix npt Self-explanatory.

Pressure control must be used with fix npt/asphere Self-explanatory.

Pressure control must be used with fix npt/body Self-explanatory.

Pressure control must be used with fix npt/sphere Self-explanatory.

Processor count in z must be 1 for 2d simulation Self-explanatory.

Processor partitions do not match number of allocated processors The total number of processors in all partitions must match the number of processors LAMMPS is running on.

Processors command after simulation box is defined The processors command cannot be used after a read_data, read_restart, or create_box command.

Processors custom grid file is inconsistent The vales in the custom file are not consistent with the number of processors you are running on or the Px,Py,Pz settings of the processors command. Or there was not a setting for every processor.

Processors grid numa and map style are incompatible Using numa for gstyle in the processors command requires using cart for the map option.

Processors part option and grid style are incompatible Cannot use gstyle numa or custom with the part option.

Processors twogrid requires proc count be a multiple of core count Self-explanatory.

Pstart and Pstop must have the same value Self-explanatory.

Python function evaluation failed The Python function did not run successfully and/or did not return a value (if it is supposed to return a value). This is probably due to some error condition in the function.

Python function is not callable The provided Python code was run successfully, but it not define a callable function with the required name.

Python invoke of undefined function Cannot invoke a function that has not been previously defined.

Python variable does not match Python function This matching is defined by the python-style variable and the python command.

Python variable has no function No python command was used to define the function associated with the python-style variable.

QEQ with 'newton pair off' not supported See the newton command. This is a restriction to use the QEQ fixes.

R0 < 0 for fix spring command Equilibrium spring length is invalid.

RATTLE coordinate constraints are not satisfied up to desired tolerance Self-explanatory.

RATTLE determinant = 0.0 The determinant of the matrix being solved for a single cluster specified by the fix rattle command is numerically invalid.

RATTLE failed Certain constraints were not satisfied.

RATTLE velocity constraints are not satisfied up to desired tolerance Self-explanatory.

Read data add offset is too big It cannot be larger than the size of atom IDs, e.g. the maximum 32-bit integer.

Read dump of atom property that isn't allocated Self-explanatory.

Read rerun dump file timestep > specified stop Self-explanatory.

Read restart MPI-IO input not allowed with % in filename This is because a % signifies one file per processor and MPI-IO creates one large file for all processors.

Read_data shrink wrap did not assign all atoms correctly This is typically because the box-size specified in the data file is large compared to the actual extent of atoms in a shrink-wrapped dimension. When LAMMPS shrink-wraps the box atoms will be lost if the processor they are re-assigned to is too far away. Choose a box size closer to the actual extent of the atoms.

Read_dump command before simulation box is defined The read_dump command cannot be used before a read_data, read_restart, or create_box command.

Read_dump field not found in dump file Self-explanatory.

Read_dump triclinic status does not match simulation Both the dump snapshot and the current LAMMPS simulation must be using either an orthogonal or triclinic box.

Read_dump xyz fields do not have consistent scaling/wrapping Self-explanatory.

Reading from MPI-IO filename when MPIIO package is not installed Self-explanatory.

Reax_defs.h setting for NATDEF is too small Edit the setting in the ReaxFF library and re-compile the library and re-build LAMMPS.

Reax_defs.h setting for NNEIGHMAXDEF is too small Edit the setting in the ReaxFF library and re-compile the library and re-build LAMMPS.

Receiving partition in processors part command is already a receiver Cannot specify a partition to be a receiver twice.

Region ID for compute chunk/atom does not exist Self-explanatory.

Region ID for compute reduce/region does not exist Self-explanatory.

Region ID for compute temp/region does not exist Self-explanatory.

Region ID for dump custom does not exist Self-explanatory.

Region ID for fix addforce does not exist Self-explanatory.

Region ID for fix atom/swap does not exist Self-explanatory.

Region ID for fix ave/spatial does not exist Self-explanatory.

Region ID for fix aveforce does not exist Self-explanatory.

Region ID for fix deposit does not exist Self-explanatory.

Region ID for fix efield does not exist Self-explanatory.

Region ID for fix evaporate does not exist Self-explanatory.

Region ID for fix gcmc does not exist Self-explanatory.

Region ID for fix heat does not exist Self-explanatory.

Region ID for fix setforce does not exist Self-explanatory.

Region ID for fix wall/region does not exist Self-explanatory.

Region ID for group dynamic does not exist Self-explanatory.

Region ID in variable formula does not exist Self-explanatory.

Region cannot have 0 length rotation vector Self-explanatory.

Region for fix oneway does not exist Self-explanatory.

Region intersect region ID does not exist Self-explanatory.

Region union or intersect cannot be dynamic The sub-regions can be dynamic, but not the combined region.

Region union region ID does not exist One or more of the region IDs specified by the region union command does not exist.

Replacing a fix, but new style != old style A fix ID can be used a 2nd time, but only if the style matches the previous fix. In this case it is assumed you with to reset a fix's parameters. This error may mean you are mistakenly re-using a fix ID when you do not intend to.

Replicate command before simulation box is defined The replicate command cannot be used before a read_data, read_restart, or create_box command.

Replicate did not assign all atoms correctly Atoms replicated by the replicate command were not assigned correctly to processors. This is likely due to some atom coordinates being outside a non-periodic simulation box.

Replicated system atom IDs are too big See the setting for tagint in the src/lmptype.h file.

Replicated system is too big See the setting for bigint in the src/lmptype.h file.

Required border comm not yet implemented with Kokkos There are various limitations in the communication options supported by Kokkos.

Rerun command before simulation box is defined The rerun command cannot be used before a read_data, read_restart, or create_box command.

Rerun dump file does not contain requested snapshot Self-explanatory.

Resetting timestep size is not allowed with fix move This is because fix move is moving atoms based on elapsed time.

Respa inner cutoffs are invalid The first cutoff must be <= the second cutoff.

Respa levels must be >= 1 Self-explanatory.

Respa middle cutoffs are invalid The first cutoff must be <= the second cutoff.

Restart file MPI-IO output not allowed with % in filename This is because a % signifies one file per processor and MPI-IO creates one large file for all processors.

Restart file byte ordering is not recognized The file does not appear to be a LAMMPS restart file since it doesn't contain a recognized byte-ordering flag at the beginning.

Restart file byte ordering is swapped The file was written on a machine with different byte-ordering than the machine you are reading it on. Convert it to a text data file instead, on the machine you wrote it on.

Restart file incompatible with current version This is probably because you are trying to read a file created with a version of LAMMPS that is too old compared to the current version. Use your older version of LAMMPS and convert the restart file to a data file.

Restart file is a MPI-IO file The file is inconsistent with the filename you specified for it.

Restart file is a multi-proc file The file is inconsistent with the filename you specified for it.

Restart file is not a MPI-IO file The file is inconsistent with the filename you specified for it.

Restart file is not a multi-proc file The file is inconsistent with the filename you specified for it.

Restart variable returned a bad timestep The variable must return a timestep greater than the current timestep.

Restrain atoms %d %d %d %d missing on proc %d at step %ld The 4 atoms in a restrain dihedral specified by the fix restrain command are not all accessible to a processor. This probably means an atom has moved too far.

Restrain atoms %d %d %d missing on proc %d at step %ld The 3 atoms in a restrain angle specified by the fix restrain command are not all accessible to a processor. This probably means an atom has moved too far.

Restrain atoms %d %d missing on proc %d at step %ld The 2 atoms in a restrain bond specified by the fix restrain command are not all accessible to a processor. This probably means an atom has moved too far.

Reuse of compute ID A compute ID cannot be used twice.

Reuse of dump ID A dump ID cannot be used twice.

Reuse of molecule template ID The template IDs must be unique.

Reuse of region ID A region ID cannot be used twice.

Rigid body atoms %d %d missing on proc %d at step %ld This means that an atom cannot find the atom that owns the rigid body it is part of, or vice versa. The solution is to use the communicate cutoff command to insure ghost atoms are acquired from far enough away to encompass the max distance printed when the fix rigid/small command was invoked.

Rigid body has degenerate moment of inertia Fix poems will only work with bodies (collections of atoms) that have non-zero principal moments of inertia. This means they must be 3 or more non-collinear atoms, even with joint atoms removed.

Rigid fix must come before NPT/NPH fix NPT/NPH fix must be defined in input script after all rigid fixes, else the rigid fix contribution to the pressure virial is incorrect.

Rmask function in equal-style variable formula Rmask is per-atom operation.

Run command before simulation box is defined The run command cannot be used before a read_data, read_restart, or create_box command.

Run command start value is after start of run Self-explanatory.

Run command stop value is before end of run Self-explanatory.

Run_style command before simulation box is defined The run_style command cannot be used before a read_data, read_restart, or create_box command.

SRD bin size for fix srd differs from user request Fix SRD had to adjust the bin size to fit the simulation box. See the cubic keyword if you want this message to be an error vs warning.

SRD bins for fix srd are not cubic enough The bin shape is not within tolerance of cubic. See the cubic keyword if you want this message to be an error vs warning.

SRD particle %d started inside big particle %d on step %ld bounce %d See the inside keyword if you want this message to be an error vs warning.

SRD particle %d started inside wall %d on step %ld bounce %d See the inside keyword if you want this message to be an error vs warning.

Same dimension twice in fix ave/spatial Self-explanatory.

Sending partition in processors part command is already a sender Cannot specify a partition to be a sender twice.

Set command before simulation box is defined The set command cannot be used before a read_data, read_restart, or create_box command.

Set command floating point vector does not exist Self-explanatory.

Set command integer vector does not exist Self-explanatory.

Set command with no atoms existing No atoms are yet defined so the set command cannot be used.

Set region ID does not exist Region ID specified in set command does not exist.

Shake angles have different bond types All 3-atom angle-constrained SHAKE clusters specified by the fix shake command that are the same angle type, must also have the same bond types for the 2 bonds in the angle.

Shake atoms %d %d %d %d missing on proc %d at step %ld The 4 atoms in a single shake cluster specified by the fix shake command are not all accessible to a processor. This probably means an atom has moved too far.

Shake atoms %d %d %d missing on proc %d at step %ld The 3 atoms in a single shake cluster specified by the fix shake command are not all accessible to a processor. This probably means an atom has moved too far.

Shake atoms %d %d missing on proc %d at step %ld The 2 atoms in a single shake cluster specified by the fix shake command are not all accessible to a processor. This probably means an atom has moved too far.

Shake cluster of more than 4 atoms A single cluster specified by the fix shake command can have no more than 4 atoms.

Shake clusters are connected A single cluster specified by the fix shake command must have a single central atom with up to 3 other atoms bonded to it.

Shake determinant = 0.0 The determinant of the matrix being solved for a single cluster specified by the fix shake command is numerically invalid.

Shake fix must come before NPT/NPH fix NPT fix must be defined in input script after SHAKE fix, else the SHAKE fix contribution to the pressure virial is incorrect.

Shear history overflow, boost neigh_modify one There are too many neighbors of a single atom. Use the neigh_modify command to increase the max number of neighbors allowed for one atom. You may also want to boost the page size.

Small to big integers are not sized correctly This error occurs when the sizes of smallint, imageint, tagint, bigint, as defined in src/lmptype.h are not what is expected. Contact the developers if this occurs.

Smallint setting in lmptype.h is invalid It has to be the size of an integer.

Smallint setting in lmptype.h is not compatible Smallint stored in restart file is not consistent with LAMMPS version you are running.

Special list size exceeded in fix bond/create See the "read_data extra/special/per/atom" command (or the "create_box extra/special/per/atom" command) for info on how to leave space in the special bonds list to allow for additional bonds to be formed.

Species XXX is not supported by this KIM Simulator Model The kim_style define command was referencing a species that is not present in the requested KIM Simulator Model.

Specified processors != physical processors The 3d grid of processors defined by the processors command does not match the number of processors LAMMPS is being run on.

Specified target stress must be uniaxial or hydrostatic Self-explanatory.

Sqrt of negative value in variable formula Self-explanatory.

Subsequent read data induced too many angles per atom See the extra/angle/per/atom keyword for the create_box or the read_data command to set this limit larger

Subsequent read data induced too many bonds per atom See the extra/bond/per/atom keyword for the create_box or the read_data command to set this limit larger

Subsequent read data induced too many dihedrals per atom See the extra/dihedral/per/atom keyword for the create_box or the read_data command to set this limit larger

Subsequent read data induced too many impropers per atom See the extra/improper/per/atom keyword for the create_box or the read_data command to set this limit larger

Substitution for illegal variable Input script line contained a variable that could not be substituted for.

Support for writing images in JPEG format not included LAMMPS was not built with the -DLAMMPS_JPEG switch in the Makefile.

Support for writing images in PNG format not included LAMMPS was not built with the -DLAMMPS_PNG switch in the Makefile.

Support for writing movies not included LAMMPS was not built with the -DLAMMPS_FFMPEG switch in the Makefile

System in data file is too big See the setting for bigint in the src/lmptype.h file.

System is not charge neutral, net charge = %g The total charge on all atoms on the system is not 0.0. For some KSpace solvers this is an error.

TAD nsteps must be multiple of t_event Self-explanatory.

TIP4P hydrogen has incorrect atom type The TIP4P pairwise computation found an H atom whose type does not agree with the specified H type.

TIP4P hydrogen is missing The TIP4P pairwise computation failed to find the correct H atom within a water molecule.

TMD target file did not list all group atoms The target file for the fix tmd command did not list all atoms in the fix group.

Tad command before simulation box is defined Self-explanatory.

Tagint setting in lmptype.h is invalid Tagint must be as large or larger than smallint.

Tagint setting in lmptype.h is not compatible Format of tagint stored in restart file is not consistent with LAMMPS version you are running. See the settings in src/lmptype.h

Target pressure for fix rigid/nph cannot be < 0.0 Self-explanatory.

Target pressure for fix rigid/npt/small cannot be < 0.0 Self-explanatory.

Target temperature for fix nvt/npt/nph cannot be 0.0 Self-explanatory.

Target temperature for fix rigid/npt cannot be 0.0 Self-explanatory.

Target temperature for fix rigid/npt/small cannot be 0.0 Self-explanatory.

Target temperature for fix rigid/nvt cannot be 0.0 Self-explanatory.

Target temperature for fix rigid/nvt/small cannot be 0.0 Self-explanatory.

Temper command before simulation box is defined The temper command cannot be used before a read_data, read_restart, or create_box command.

Temperature ID for fix bond/swap does not exist Self-explanatory.

Temperature ID for fix box/relax does not exist Self-explanatory.

Temperature ID for fix nvt/npt does not exist Self-explanatory.

Temperature ID for fix press/berendsen does not exist Self-explanatory.

Temperature ID for fix rigid nvt/npt/nph does not exist Self-explanatory.

Temperature ID for fix temp/berendsen does not exist Self-explanatory.

Temperature ID for fix temp/csld does not exist Self-explanatory.

Temperature ID for fix temp/csvr does not exist Self-explanatory.

Temperature ID for fix temp/rescale does not exist Self-explanatory.

Temperature compute degrees of freedom < 0 This should not happen if you are calculating the temperature on a valid set of atoms.

Temperature control can not be used with fix nph Self-explanatory.

Temperature control can not be used with fix nph/asphere Self-explanatory.

Temperature control can not be used with fix nph/body Self-explanatory.

Temperature control can not be used with fix nph/sphere Self-explanatory.

Temperature control must be used with fix nphug The temp keyword must be provided.

Temperature control must be used with fix npt Self-explanatory.

Temperature control must be used with fix npt/asphere Self-explanatory.

Temperature control must be used with fix npt/body Self-explanatory.

Temperature control must be used with fix npt/sphere Self-explanatory.

Temperature control must be used with fix nvt Self-explanatory.

Temperature control must be used with fix nvt/asphere Self-explanatory.

Temperature control must be used with fix nvt/body Self-explanatory.

Temperature control must be used with fix nvt/sllod Self-explanatory.

Temperature control must be used with fix nvt/sphere Self-explanatory.

Temperature control must not be used with fix nph/small Self-explanatory.

Temperature for fix nvt/sllod does not have a bias The specified compute must compute temperature with a bias.

Tempering could not find thermo_pe compute This compute is created by the thermo command. It must have been explicitly deleted by a uncompute command.

Tempering fix ID is not defined The fix ID specified by the temper command does not exist.

Tempering temperature fix is not valid The fix specified by the temper command is not one that controls temperature (nvt or langevin).

Test_descriptor_string already allocated This is an internal error. Contact the developers.

The package gpu command is required for gpu styles Self-explanatory.

Thermo and fix not computed at compatible times Fixes generate values on specific timesteps. The thermo output does not match these timesteps.

Thermo compute array is accessed out-of-range Self-explanatory.

Thermo compute does not compute array Self-explanatory.

Thermo compute does not compute scalar Self-explanatory.

Thermo compute does not compute vector Self-explanatory.

Thermo compute vector is accessed out-of-range Self-explanatory.

Thermo custom variable cannot be indexed Self-explanatory.

Thermo custom variable is not equal-style variable Only equal-style variables can be output with thermodynamics, not atom-style variables.

Thermo every variable returned a bad timestep The variable must return a timestep greater than the current timestep.

Thermo fix array is accessed out-of-range Self-explanatory.

Thermo fix does not compute array Self-explanatory.

Thermo fix does not compute scalar Self-explanatory.

Thermo fix does not compute vector Self-explanatory.

Thermo fix vector is accessed out-of-range Self-explanatory.

Thermo keyword in variable requires thermo to use/init pe You are using a thermo keyword in a variable that requires potential energy to be calculated, but your thermo output does not use it. Add it to your thermo output.

Thermo keyword in variable requires thermo to use/init press You are using a thermo keyword in a variable that requires pressure to be calculated, but your thermo output does not use it. Add it to your thermo output.

Thermo keyword in variable requires thermo to use/init temp You are using a thermo keyword in a variable that requires temperature to be calculated, but your thermo output does not use it. Add it to your thermo output.

Thermo style does not use press Cannot use thermo_modify to set this parameter since the thermo_style is not computing this quantity.

Thermo style does not use temp Cannot use thermo_modify to set this parameter since the thermo_style is not computing this quantity.

Thermo_modify every variable returned a bad timestep The returned timestep is less than or equal to the current timestep.

Thermo_modify int format does not contain d character Self-explanatory.

Thermo_modify pressure ID does not compute pressure The specified compute ID does not compute pressure.

Thermo_modify temperature ID does not compute temperature The specified compute ID does not compute temperature.

Thermo_style command before simulation box is defined The thermo_style command cannot be used before a read_data, read_restart, or create_box command.

This variable thermo keyword cannot be used between runs Keywords that refer to time (such as cpu, elapsed) do not make sense in between runs.

Threshhold for an atom property that isn't allocated A dump threshold has been requested on a quantity that is not defined by the atom style used in this simulation.

Timestep must be >= 0 Specified timestep is invalid.

Too big a problem to use velocity create loop all The system size must fit in a 32-bit integer to use this option.

Too big a timestep for dump dcd The timestep must fit in a 32-bit integer to use this dump style.

Too big a timestep for dump xtc The timestep must fit in a 32-bit integer to use this dump style.

Too few bits for lookup table Table size specified via pair_modify command does not work with your machine's floating point representation.

Too few lines in %s section of data file Self-explanatory.

Too few values in body lines in data file Self-explanatory.

Too few values in body section of molecule file Self-explanatory.

Too many -pk arguments in command line The string formed by concatenating the arguments is too long. Use a package command in the input script instead.

Too many MSM grid levels The max number of MSM grid levels is hardwired to 10.

Too many args in variable function More args are used than any variable function allows.

Too many atom pairs for pair bop The number of atomic pairs exceeds the expected number. Check your atomic structure to ensure that it is realistic.

Too many atom sorting bins This is likely due to an immense simulation box that has blown up to a large size.

Too many atom triplets for pair bop The number of three atom groups for angle determinations exceeds the expected number. Check your atomic structure to ensure that it is realistic.

Too many atoms for dump dcd The system size must fit in a 32-bit integer to use this dump style.

Too many atoms for dump xtc The system size must fit in a 32-bit integer to use this dump style.

Too many atoms to dump sort Cannot sort when running with more than 2^31 atoms.

Too many exponent bits for lookup table Table size specified via pair_modify command does not work with your machine's floating point representation.

Too many groups The maximum number of atom groups (including the "all" group) is given by MAX_GROUP in group.cpp and is 32.

Too many iterations You must use a number of iterations that fit in a 32-bit integer for minimization.

Too many lines in one body in data file - boost MAXBODY MAXBODY is a setting at the top of the src/read_data.cpp file. Set it larger and re-compile the code.

Too many local+ghost atoms for neighbor list The number of nlocal + nghost atoms on a processor is limited by the size of a 32-bit integer with 2 bits removed for masking 1-2, 1-3, 1-4 neighbors.

Too many mantissa bits for lookup table Table size specified via pair_modify command does not work with your machine's floating point representation.

Too many masses for fix shake The fix shake command cannot list more masses than there are atom types.

Too many molecules for fix poems The limit is 2^31 = ~2 billion molecules.

Too many molecules for fix rigid The limit is 2^31 = ~2 billion molecules.

Too many neighbor bins This is likely due to an immense simulation box that has blown up to a large size.

Too many timesteps The cumulative timesteps must fit in a 64-bit integer.

Too many timesteps for NEB You must use a number of timesteps that fit in a 32-bit integer for NEB.

Too many total atoms See the setting for bigint in the src/lmptype.h file.

Too many total bits for bitmapped lookup table Table size specified via pair_modify command is too large. Note that a value of N generates a 2^N size table.

Too many values in body lines in data file Self-explanatory.

Too many values in body section of molecule file Self-explanatory.

Too much buffered per-proc info for dump The size of the buffered string must fit in a 32-bit integer for a dump.

Too much per-proc info for dump Number of local atoms times number of columns must fit in a 32-bit integer for dump.

Tree structure in joint connections Fix poems cannot (yet) work with coupled bodies whose joints connect the bodies in a tree structure.

Triclinic box skew is too large The displacement in a skewed direction must be less than half the box length in that dimension. E.g. the xy tilt must be between -half and +half of the x box length. This constraint can be relaxed by using the box tilt command.

Tried to convert a double to int, but input_double > INT_MAX Self-explanatory.

Trying to build an occasional neighbor list before initialization completed This is not allowed. Source code caller needs to be modified.

Two fix ave commands using same compute chunk/atom command in incompatible ways They are both attempting to "lock" the chunk/atom command so that the chunk assignments persist for some number of timesteps, but are doing it in different ways.

Two groups cannot be the same in fix spring couple Self-explanatory.

Unable to initialize accelerator for use There was a problem initializing an accelerator for the gpu package

Unbalanced quotes in input line No matching end double quote was found following a leading double quote.

Unexpected end of -reorder file Self-explanatory.

Unexpected empty line in AngleCoeffs section Read a blank line where there should be coefficient data.

Unexpected empty line in BondCoeffs section Read a blank line where there should be coefficient data.

Unexpected empty line in DihedralCoeffs section Read a blank line where there should be coefficient data.

Unexpected empty line in ImproperCoeffs section Read a blank line where there should be coefficient data.

Unexpected empty line in PairCoeffs section Read a blank line where there should be coefficient data.

Unexpected end of custom file Self-explanatory.

Unexpected end of data file LAMMPS hit the end of the data file while attempting to read a section. Something is wrong with the format of the data file.

Unexpected end of dump file A read operation from the file failed.

Unexpected end of fix rigid file A read operation from the file failed.

Unexpected end of fix rigid/small file A read operation from the file failed.

Unexpected end of molecule file Self-explanatory.

Unexpected end of neb file A read operation from the file failed.

Units command after simulation box is defined The units command cannot be used after a read_data, read_restart, or create_box command.

Universe/uloop variable count < # of partitions A universe or uloop style variable must specify a number of values >= to the number of processor partitions.

Unrecognized angle style The choice of angle style is unknown.

Unrecognized atom style The choice of atom style is unknown.

Unrecognized body style The choice of body style is unknown.

Unrecognized bond style The choice of bond style is unknown.

Unknown category for info is_active() Self-explanatory.

Unknown category for info is_available() Self-explanatory.

Unknown category for info is_defined() Self-explanatory.

Unrecognized command: %s The command is not known to LAMMPS. Check the input script.

Unrecognized compute style The choice of compute style is unknown.

Unrecognized dihedral style The choice of dihedral style is unknown.

Unrecognized dump reader style The choice of dump reader style via the format keyword is unknown.

Unrecognized dump style The choice of dump style is unknown.

Unknown error in GPU library Self-explanatory.

Unrecognized fix style The choice of fix style is unknown.

Unknown identifier in data file: %s A section of the data file cannot be read by LAMMPS.

Unrecognized improper style The choice of improper style is unknown.

Unknown keyword in thermo_style custom command One or more specified keywords are not recognized.

Unrecognized kspace style The choice of kspace style is unknown.

Unknown name for info newton category Self-explanatory.

Unknown name for info package category Self-explanatory.

Unknown name for info pair category Self-explanatory.

Unrecognized pair style The choice of pair style is unknown.

Unknown pair_modify hybrid sub-style The choice of sub-style is unknown.

Unrecognized region style The choice of region style is unknown.

Unknown section in molecule file Self-explanatory.

Unknown table style in angle style table Self-explanatory.

Unknown table style in bond style table Self-explanatory.

Unknown table style in pair_style command Style of table is invalid for use with pair_style table command.

Unknown unit_style Self-explanatory. Check the input script or data file.

Unrecognized lattice type in MEAM file 1 The lattice type in an entry of the MEAM library file is not valid.

Unrecognized lattice type in MEAM file 2 The lattice type in an entry of the MEAM parameter file is not valid.

Unrecognized pair style in compute pair command Self-explanatory.

Unsupported mixing rule in kspace_style ewald/disp Only geometric mixing is supported.

Unsupported order in kspace_style ewald/disp Only 1/r^6 dispersion or dipole terms are supported.

Unsupported order in kspace_style pppm/disp, pair_style %s Only pair styles with 1/r and 1/r^6 dependence are currently supported.

Use cutoff keyword to set cutoff in single mode Mode is single so cutoff/multi keyword cannot be used.

Use cutoff/multi keyword to set cutoff in multi mode Mode is multi so cutoff keyword cannot be used.

Using fix nvt/sllod with inconsistent fix deform remap option Fix nvt/sllod requires that deforming atoms have a velocity profile provided by "remap v" as a fix deform option.

Using fix nvt/sllod with no fix deform defined Self-explanatory.

Using fix srd with inconsistent fix deform remap option When shearing the box in an SRD simulation, the remap v option for fix deform needs to be used.

Using pair lubricate with inconsistent fix deform remap option Must use remap v option with fix deform with this pair style.

Using pair lubricate/poly with inconsistent fix deform remap option If fix deform is used, the remap v option is required.

Using suffix gpu without GPU package installed Self-explanatory.

Using suffix intel without USER-INTEL package installed Self-explanatory.

Using suffix kk without KOKKOS package enabled Self-explanatory.

Using suffix omp without USER-OMP package installed Self-explanatory.

Using update dipole flag requires atom attribute mu Self-explanatory.

Using update dipole flag requires atom style sphere Self-explanatory.

Variable ID in variable formula does not exist Self-explanatory.

Variable atom ID is too large Specified ID is larger than the maximum allowed atom ID.

Variable evaluation before simulation box is defined Cannot evaluate a compute or fix or atom-based value in a variable before the simulation has been setup.

Variable evaluation in fix wall gave bad value The returned value for epsilon or sigma < 0.0.

Variable evaluation in region gave bad value Variable returned a radius < 0.0.

Variable for compute ti is invalid style Self-explanatory.

Variable for create_atoms is invalid style The variables must be equal-style variables.

Variable for displace_atoms is invalid style It must be an equal-style or atom-style variable.

Variable for dump every is invalid style Only equal-style variables can be used.

Variable for dump image center is invalid style Must be an equal-style variable.

Variable for dump image persp is invalid style Must be an equal-style variable.

Variable for dump image phi is invalid style Must be an equal-style variable.

Variable for dump image theta is invalid style Must be an equal-style variable.

Variable for dump image zoom is invalid style Must be an equal-style variable.

Variable for fix adapt is invalid style Only equal-style variables can be used.

Variable for fix addforce is invalid style Self-explanatory.

Variable for fix aveforce is invalid style Only equal-style variables can be used.

Variable for fix deform is invalid style The variable must be an equal-style variable.

Variable for fix efield is invalid style The variable must be an equal- or atom-style variable.

Variable for fix gravity is invalid style Only equal-style variables can be used.

Variable for fix heat is invalid style Only equal-style or atom-style variables can be used.

Variable for fix indent is invalid style Only equal-style variables can be used.

Variable for fix indent is not equal style Only equal-style variables can be used.

Variable for fix langevin is invalid style It must be an equal-style variable.

Variable for fix move is invalid style Only equal-style variables can be used.

Variable for fix setforce is invalid style Only equal-style variables can be used.

Variable for fix temp/berendsen is invalid style Only equal-style variables can be used.

Variable for fix temp/csld is invalid style Only equal-style variables can be used.

Variable for fix temp/csvr is invalid style Only equal-style variables can be used.

Variable for fix temp/rescale is invalid style Only equal-style variables can be used.

Variable for fix wall is invalid style Only equal-style variables can be used.

Variable for fix wall/reflect is invalid style Only equal-style variables can be used.

Variable for fix wall/srd is invalid style Only equal-style variables can be used.

Variable for group dynamic is invalid style The variable must be an atom-style variable.

Variable for group is invalid style Only atom-style variables can be used.

Variable for region cylinder is invalid style Only equal-style variables are allowed.

Variable for region is invalid style Only equal-style variables can be used.

Variable for region is not equal style Self-explanatory.

Variable for region sphere is invalid style Only equal-style variables are allowed.

Variable for restart is invalid style Only equal-style variables can be used.

Variable for set command is invalid style Only atom-style variables can be used.

Variable for thermo every is invalid style Only equal-style variables can be used.

Variable for velocity set is invalid style Only atom-style variables can be used.

Variable for voronoi radius is not atom style Self-explanatory.

Variable formula compute array is accessed out-of-range Self-explanatory.

Variable formula compute vector is accessed out-of-range Self-explanatory.

Variable formula fix array is accessed out-of-range Self-explanatory.

Variable formula fix vector is accessed out-of-range Self-explanatory.

Variable has circular dependency A circular dependency is when variable "a" in used by variable "b" and variable "b" is also used by variable "a". Circular dependencies with longer chains of dependence are also not allowed.

Variable name between brackets must be alphanumeric or underscore characters Self-explanatory.

Variable name for compute chunk/atom does not exist Self-explanatory.

Variable name for compute reduce does not exist Self-explanatory.

Variable name for compute ti does not exist Self-explanatory.

Variable name for create_atoms does not exist Self-explanatory.

Variable name for displace_atoms does not exist Self-explanatory.

Variable name for dump every does not exist Self-explanatory.

Variable name for dump image center does not exist Self-explanatory.

Variable name for dump image persp does not exist Self-explanatory.

Variable name for dump image phi does not exist Self-explanatory.

Variable name for dump image theta does not exist Self-explanatory.

Variable name for dump image zoom does not exist Self-explanatory.

Variable name for fix adapt does not exist Self-explanatory.

Variable name for fix addforce does not exist Self-explanatory.

Variable name for fix ave/atom does not exist Self-explanatory.

Variable name for fix ave/chunk does not exist Self-explanatory.

Variable name for fix ave/correlate does not exist Self-explanatory.

Variable name for fix ave/histo does not exist Self-explanatory.

Variable name for fix ave/spatial does not exist Self-explanatory.

Variable name for fix ave/time does not exist Self-explanatory.

Variable name for fix aveforce does not exist Self-explanatory.

Variable name for fix deform does not exist Self-explanatory.

Variable name for fix efield does not exist Self-explanatory.

Variable name for fix gravity does not exist Self-explanatory.

Variable name for fix heat does not exist Self-explanatory.

Variable name for fix indent does not exist Self-explanatory.

Variable name for fix langevin does not exist Self-explanatory.

Variable name for fix move does not exist Self-explanatory.

Variable name for fix setforce does not exist Self-explanatory.

Variable name for fix store/state does not exist Self-explanatory.

Variable name for fix temp/berendsen does not exist Self-explanatory.

Variable name for fix temp/csld does not exist Self-explanatory.

Variable name for fix temp/csvr does not exist Self-explanatory.

Variable name for fix temp/rescale does not exist Self-explanatory.

Variable name for fix vector does not exist Self-explanatory.

Variable name for fix wall does not exist Self-explanatory.

Variable name for fix wall/reflect does not exist Self-explanatory.

Variable name for fix wall/srd does not exist Self-explanatory.

Variable name for group does not exist Self-explanatory.

Variable name for group dynamic does not exist Self-explanatory.

Variable name for region cylinder does not exist Self-explanatory.

Variable name for region does not exist Self-explanatory.

Variable name for region sphere does not exist Self-explanatory.

Variable name for restart does not exist Self-explanatory.

Variable name for set command does not exist Self-explanatory.

Variable name for thermo every does not exist Self-explanatory.

Variable name for velocity set does not exist Self-explanatory.

Variable name for voronoi radius does not exist Self-explanatory.

Variable name must be alphanumeric or underscore characters Self-explanatory.

Variable uses atom property that isn't allocated Self-explanatory.

Velocity command before simulation box is defined The velocity command cannot be used before a read_data, read_restart, or create_box command.

Velocity command with no atoms existing A velocity command has been used, but no atoms yet exist.

Velocity ramp in z for a 2d problem Self-explanatory.

Velocity rigid used with non-rigid fix-ID Self-explanatory.

Velocity temperature ID does calculate a velocity bias The specified compute must compute a bias for temperature.

Velocity temperature ID does not compute temperature The compute ID given to the velocity command must compute temperature.

Verlet/split can only currently be used with comm_style brick This is a current restriction in LAMMPS.

Verlet/split does not yet support TIP4P This is a current limitation.

Verlet/split requires 2 partitions See the -partition command-line switch.

Verlet/split requires Rspace partition layout be multiple of Kspace partition layout in each dim This is controlled by the processors command.

Verlet/split requires Rspace partition size be multiple of Kspace partition size This is so there is an equal number of Rspace processors for every Kspace processor.

Virial was not tallied on needed timestep You are using a thermo keyword that requires potentials to have tallied the virial, but they didn't on this timestep. See the variable doc page for ideas on how to make this work.

Voro++ error: narea and neigh have a different size This error is returned by the Voro++ library.

Wall defined twice in fix wall command Self-explanatory.

Wall defined twice in fix wall/reflect command Self-explanatory.

Wall defined twice in fix wall/srd command Self-explanatory.

Water H epsilon must be 0.0 for pair style lj/cut/tip4p/cut This is because LAMMPS does not compute the Lennard-Jones interactions with these particles for efficiency reasons.

Water H epsilon must be 0.0 for pair style lj/cut/tip4p/long This is because LAMMPS does not compute the Lennard-Jones interactions with these particles for efficiency reasons.

Water H epsilon must be 0.0 for pair style lj/long/tip4p/long This is because LAMMPS does not compute the Lennard-Jones interactions with these particles for efficiency reasons.

World variable count doesn't match # of partitions A world-style variable must specify a number of values equal to the number of processor partitions.

Write_data command before simulation box is defined Self-explanatory.

Write_restart command before simulation box is defined The write_restart command cannot be used before a read_data, read_restart, or create_box command.

Writing to MPI-IO filename when MPIIO package is not installed Self-explanatory.

Zero length rotation vector with displace_atoms Self-explanatory.

Zero length rotation vector with fix move Self-explanatory.

Zero-length lattice orient vector Self-explanatory.

13.4 Warning messages

This is an alphabetic list of the WARNING messages LAMMPS prints out and the reason why. If the explanation here is not sufficient, the documentation for the offending command may help. Warning messages also list the source file and line number where the warning was generated. For example, a message like this:

```
WARNING: Bond atom missing in box size check (domain.cpp:187)
```

means that line #187 in the file src/domain.cpp generated the error. Looking in the source code may help you figure out what went wrong.

Note that warning messages from *user-contributed packages* are not listed here. If such a warning occurs and is not self-explanatory, you will need to look in the source code or contact the author of the package.

Doc page with *ERROR messages*

Adjusting Coulombic cutoff for MSM, new cutoff = %g The adjust/cutoff command is turned on and the Coulombic cutoff has been adjusted to match the user-specified accuracy.

Angle atoms missing at step %ld One or more of 3 atoms needed to compute a particular angle are missing on this processor. Typically this is because the pairwise cutoff is set too short or the angle has blown apart and an atom is too far away.

Angle style in data file differs from currently defined angle style Self-explanatory.

Angles are defined but no angle style is set The topology contains angles, but there are no angle forces computed since there was no angle_style command.

Atom style in data file differs from currently defined atom style Self-explanatory.

Bond atom missing in box size check The 2nd atoms needed to compute a particular bond is missing on this processor. Typically this is because the pairwise cutoff is set too short or the bond has blown apart and an atom is too far away.

Bond atom missing in image check The 2nd atom in a particular bond is missing on this processor. Typically this is because the pairwise cutoff is set too short or the bond has blown apart and an atom is too far away.

Bond atoms missing at step %ld The 2nd atom needed to compute a particular bond is missing on this processor. Typically this is because the pairwise cutoff is set too short or the bond has blown apart and an atom is too far away.

Bond style in data file differs from currently defined bond style Self-explanatory.

Bonds are defined but no bond style is set The topology contains bonds, but there are no bond forces computed since there was no bond_style command.

Bond/angle/dihedral extent > half of periodic box length This is a restriction because LAMMPS can be confused about which image of an atom in the bonded interaction is the correct one to use. "Extent" in this context means the maximum end-to-end length of the bond/angle/dihedral. LAMMPS computes this by taking the maximum bond length, multiplying by the number of bonds in the interaction (e.g. 3 for a dihedral) and adding a small amount of stretch.

Bond/react: Atom affected by reaction too close to template edge This means an atom which changes type or connectivity during the reaction is too close to an 'edge' atom defined in the superimpose file. This could cause incorrect assignment of bonds, angle, etc. Generally, this means you must include more atoms in your templates, such that there are at least two atoms between each atom involved in the reaction and an edge atom.

Both groups in compute group/group have a net charge; the Kspace boundary correction to energy will be non-zero Self-explanatory.

Calling write_dump before a full system init. The write_dump command is used before the system has been fully initialized as part of a 'run' or 'minimize' command. Not all dump styles and features are fully supported at this point and thus the command may fail or produce incomplete or incorrect output. Insert a "run 0" command, if a full system init is required.

Cannot count rigid body degrees-of-freedom before bodies are fully initialized This means the temperature associated with the rigid bodies may be incorrect on this timestep.

Cannot count rigid body degrees-of-freedom before bodies are initialized This means the temperature associated with the rigid bodies may be incorrect on this timestep.

Cannot include log terms without 1/r terms; setting flagHI to 1 Self-explanatory.

Cannot include log terms without 1/r terms; setting flagHI to 1. Self-explanatory.

Charges are set, but coulombic solver is not used Self-explanatory.

Charges did not converge at step %ld: %lg Self-explanatory.

Communication cutoff is 0.0. No ghost atoms will be generated. Atoms may get lost The communication cutoff defaults to the maximum of what is inferred from pair and bond styles (will be zero, if none are defined) and what is specified via *comm_modify cutoff* (defaults to 0.0). If this results to 0.0, no ghost atoms will be generated and

LAMMPS may lose atoms or use incorrect periodic images of atoms in interaction lists. To avoid, either use *pair style zero* with a suitable cutoff or use *comm_modify cutoff*.

Communication cutoff is too small for SNAP micro load balancing, increased to %lf Self-explanatory.

Compute cna/atom cutoff may be too large to find ghost atom neighbors The neighbor cutoff used may not encompass enough ghost atoms to perform this operation correctly.

Computing temperature of portions of rigid bodies The group defined by the temperature compute does not encompass all the atoms in one or more rigid bodies, so the change in degrees-of-freedom for the atoms in those partial rigid bodies will not be accounted for.

Create_bonds max distance > minimum neighbor cutoff This means atom pairs for some atom types may not be in the neighbor list and thus no bond can be created between them.

Delete_atoms cutoff > minimum neighbor cutoff This means atom pairs for some atom types may not be in the neighbor list and thus an atom in that pair cannot be deleted.

Dihedral atoms missing at step %ld One or more of 4 atoms needed to compute a particular dihedral are missing on this processor. Typically this is because the pairwise cutoff is set too short or the dihedral has blown apart and an atom is too far away.

Dihedral problem Conformation of the 4 listed dihedral atoms is extreme; you may want to check your simulation geometry.

Dihedral problem: %d %ld %d %d %d %d Conformation of the 4 listed dihedral atoms is extreme; you may want to check your simulation geometry.

Dihedral style in data file differs from currently defined dihedral style Self-explanatory.

Dihedrals are defined but no dihedral style is set The topology contains dihedrals, but there are no dihedral forces computed since there was no dihedral_style command.

Dump dcd/xtc timestamp may be wrong with fix dt/reset If the fix changes the timestep, the dump dcd file will not reflect the change.

Energy due to X extra global DOFs will be included in minimizer energies When using fixes like box/relax, the potential energy used by the minimizer is augmented by an additional energy provided by the fix. Thus the printed converged energy may be different from the total potential energy.

Estimated error in splitting of dispersion coeffs is %g Error is greater than 0.0001 percent.

Ewald/disp Newton solver failed, using old method to estimate g_ewald Self-explanatory. Choosing a different cutoff value may help.

FENE bond too long A FENE bond has stretched dangerously far. It's interaction strength will be truncated to attempt to prevent the bond from blowing up.

FENE bond too long: %ld %d %d %g A FENE bond has stretched dangerously far. It's interaction strength will be truncated to attempt to prevent the bond from blowing up.

FENE bond too long: %ld %g A FENE bond has stretched dangerously far. It's interaction strength will be truncated to attempt to prevent the bond from blowing up.

Fix SRD walls overlap but fix srd overlap not set You likely want to set this in your input script.

- **Fix bond/create is used multiple times or with fix bond/break - may not work as expected*** When using fix bond/create multiple times or in combination with fix bond/break, the individual fix instances do not share information about changes they made at the same time step and thus it may result in unexpected behavior.

Fix bond/swap will ignore defined angles See the doc page for fix bond/swap for more info on this restriction.

Fix deposit near setting < possible overlap separation %g This test is performed for finite size particles with a diameter, not for point particles. The near setting is smaller than the particle diameter which can lead to overlaps.

Fix evaporate may delete atom with non-zero molecule ID This is probably an error, since you should not delete only one atom of a molecule.

Fix gcmc using full_energy option Fix gcmc has automatically turned on the full_energy option since it is required for systems like the one specified by the user. User input included one or more of the following: kspace, triclinic, a hybrid pair style, an eam pair style, or no "single" function for the pair style.

Fix langevin gjf using random gaussians is not implemented with kokkos This will most likely cause errors in kinetic fluctuations.

Fix property/atom mol or charge w/out ghost communication A model typically needs these properties defined for ghost atoms.

Fix qeq CG convergence failed (%g) after %d iterations at %ld step Self-explanatory.

Fix qeq has non-zero lower Taper radius cutoff Absolute value must be <= 0.01.

Fix qeq has very low Taper radius cutoff Value should typically be >= 5.0.

Fix qeq/dynamic tolerance may be too small for damped dynamics Self-explanatory.

Fix qeq/fire tolerance may be too small for damped fires Self-explanatory.

Fix rattle should come after all other integration fixes This fix is designed to work after all other integration fixes change atom positions. Thus it should be the last integration fix specified. If not, it will not satisfy the desired constraints as well as it otherwise would.

Fix recenter should come after all other integration fixes Other fixes may change the position of the center-of-mass, so fix recenter should come last.

Fix srd SRD moves may trigger frequent reneighboring This is because the SRD particles may move long distances.

Fix srd grid size > 1/4 of big particle diameter This may cause accuracy problems.

Fix srd particle moved outside valid domain This may indicate a problem with your simulation parameters.

Fix srd particles may move > big particle diameter This may cause accuracy problems.

Fix srd viscosity < 0.0 due to low SRD density This may cause accuracy problems.

Fixes cannot send data in Kokkos communication, switching to classic communication This is current restriction with Kokkos.

For better accuracy use 'pair_modify table 0' The user-specified force accuracy cannot be achieved unless the table feature is disabled by using 'pair_modify table 0'.

Geometric mixing assumed for 1/r^6 coefficients Self-explanatory.

Group for fix_modify temp != fix group The fix_modify command is specifying a temperature computation that computes a temperature on a different group of atoms than the fix itself operates on. This is probably not what you want to do.

H matrix size has been exceeded: m_fill=%d H.m=%dn This is the size of the matrix.

Ignoring unknown or incorrect info command flag Self-explanatory. An unknown argument was given to the info command. Compare your input with the documentation.

Improper atoms missing at step %ld One or more of 4 atoms needed to compute a particular improper are missing on this processor. Typically this is because the pairwise cutoff is set too short or the improper has blown apart and an atom is too far away.

Improper problem: %d %ld %d %d %d %d Conformation of the 4 listed improper atoms is extreme; you may want to check your simulation geometry.

Improper style in data file differs from currently defined improper style Self-explanatory.

Impropers are defined but no improper style is set The topology contains impropers, but there are no improper forces computed since there was no improper_style command.

Inconsistent image flags The image flags for a pair on bonded atoms appear to be inconsistent. Inconsistent means that when the coordinates of the two atoms are unwrapped using the image flags, the two atoms are far apart. Specifically they are further apart than half a periodic box length. Or they are more than a box length apart in a non-periodic dimension. This is usually due to the initial data file not having correct image flags for the 2 atoms in a bond that straddles a periodic boundary. They should be different by 1 in that case. This is a warning because inconsistent image flags will not cause problems for dynamics or most LAMMPS simulations. However they can cause problems when such atoms are used with the fix rigid or replicate commands. Note that if you have an infinite periodic crystal with bonds then it is impossible to have fully consistent image flags, since some bonds will cross periodic boundaries and connect two atoms with the same image flag.

Increasing communication cutoff for GPU style The pair style has increased the communication cutoff to be consistent with the communication cutoff requirements for this pair style when run on the GPU.

KIM Model does not provide 'energy'; Potential energy will be zero Self-explanatory.

KIM Model does not provide 'forces'; Forces will be zero Self-explanatory.

KIM Model does not provide 'particleEnergy'; energy per atom will be zero Self-explanatory.

KIM Model does not provide 'particleVirial'; virial per atom will be zero Self-explanatory.

Kspace_modify slab param < 2.0 may cause unphysical behavior The kspace_modify slab parameter should be larger to insure periodic grids padded with empty space do not overlap.

Less insertions than requested The fix pour command was unsuccessful at finding open space for as many particles as it tried to insert.

Library error in lammps_gather_atoms This library function cannot be used if atom IDs are not defined or are not consecutively numbered.

Library error in lammps_scatter_atoms This library function cannot be used if atom IDs are not defined or are not consecutively numbered, or if no atom map is defined. See the atom_modify command for details about atom maps.

Likewise 1-2 special neighbor interactions != 1.0 The topology contains bonds, but there is no bond style defined and a 1-2 special neighbor scaling factor was not 1.0. This means that pair style interactions may have scaled or missing pairs in the neighbor list in expectation of interactions for those pairs being computed from the bond style.

Likewise 1-3 special neighbor interactions != 1.0 The topology contains angles, but there is no angle style defined and a 1-3 special neighbor scaling factor was not 1.0. This means that pair style interactions may have scaled or missing pairs in the neighbor list in expectation of interactions for those pairs being computed from the angle style.

Likewise 1-4 special neighbor interactions != 1.0 The topology contains dihedrals, but there is no dihedral style defined and a 1-4 special neighbor scaling factor was not 1.0. This means that pair style interactions may have scaled or missing pairs in the neighbor list in expectation of interactions for those pairs being computed from the dihedral style.

Lost atoms via change_box: original %ld current %ld The command options you have used caused atoms to be lost.

Lost atoms via displace_atoms: original %ld current %ld The command options you have used caused atoms to be lost.

Lost atoms: original %ld current %ld Lost atoms are checked for each time thermo output is done. See the thermo_modify lost command for options. Lost atoms usually indicate bad dynamics, e.g. atoms have been

blown far out of the simulation box, or moved further than one processor's sub-domain away before reneighboring.

MSM mesh too small, increasing to 2 points in each direction Self-explanatory.

Mismatch between velocity and compute groups The temperature computation used by the velocity command will not be on the same group of atoms that velocities are being set for.

Mixing forced for lj coefficients Self-explanatory.

Molecule attributes do not match system attributes An attribute is specified (e.g. diameter, charge) that is not defined for the specified atom style.

Molecule has bond topology but no special bond settings This means the bonded atoms will not be excluded in pairwise interactions.

Molecule template for create_atoms has multiple molecules The create_atoms command will only create molecules of a single type, i.e. the first molecule in the template.

Molecule template for fix gcmc has multiple molecules The fix gcmc command will only create molecules of a single type, i.e. the first molecule in the template.

Molecule template for fix shake has multiple molecules The fix shake command will only recognize molecules of a single type, i.e. the first molecule in the template.

More than one compute centro/atom It is not efficient to use compute centro/atom more than once.

More than one compute cluster/atom It is not efficient to use compute cluster/atom more than once.

More than one compute cna/atom defined It is not efficient to use compute cna/atom more than once.

More than one compute contact/atom It is not efficient to use compute contact/atom more than once.

More than one compute coord/atom It is not efficient to use compute coord/atom more than once.

More than one compute damage/atom It is not efficient to use compute ke/atom more than once.

More than one compute dilatation/atom Self-explanatory.

More than one compute erotate/sphere/atom It is not efficient to use compute erorate/sphere/atom more than once.

More than one compute hexorder/atom It is not efficient to use compute hexorder/atom more than once.

More than one compute ke/atom It is not efficient to use compute ke/atom more than once.

More than one compute orientorder/atom It is not efficient to use compute orientorder/atom more than once.

More than one compute plasticity/atom Self-explanatory.

More than one compute sna/atom Self-explanatory.

More than one compute snad/atom Self-explanatory.

More than one compute snav/atom Self-explanatory.

More than one fix poems It is not efficient to use fix poems more than once.

More than one fix rigid It is not efficient to use fix rigid more than once.

Neighbor exclusions used with KSpace solver may give inconsistent Coulombic energies This is because excluding specific pair interactions also excludes them from long-range interactions which may not be the desired effect. The special_bonds command handles this consistently by insuring excluded (or weighted) 1-2, 1-3, 1-4 interactions are treated consistently by both the short-range pair style and the long-range solver. This is not done for exclusions of charged atom pairs via the neigh_modify exclude command.

New thermo_style command, previous thermo_modify settings will be lost If a thermo_style command is used after a thermo_modify command, the settings changed by the thermo_modify command will be reset to their default values. This is because the thermo_modify command acts on the currently defined thermo style, and a thermo_style command creates a new style.

No Kspace calculation with verlet/split The 2nd partition performs a kspace calculation so the kspace_style command must be used.

No automatic unit conversion to XTC file format conventions possible for units lj This means no scaling will be performed.

No fixes defined, atoms won't move If you are not using a fix like nve, nvt, npt then atom velocities and coordinates will not be updated during timestepping.

No joints between rigid bodies, use fix rigid instead The bodies defined by fix poems are not connected by joints. POEMS will integrate the body motion, but it would be more efficient to use fix rigid.

Not using real units with pair reax This is most likely an error, unless you have created your own ReaxFF parameter file in a different set of units.

Number of MSM mesh points changed to be a multiple of 2 MSM requires that the number of grid points in each direction be a multiple of two and the number of grid points in one or more directions have been adjusted to meet this requirement.

OMP_NUM_THREADS environment is not set. This environment variable must be set appropriately to use the USER-OMP package.

One or more atoms are time integrated more than once This is probably an error since you typically do not want to advance the positions or velocities of an atom more than once per timestep.

One or more chunks do not contain all atoms in molecule This may not be what you intended.

One or more dynamic groups may not be updated at correct point in timestep If there are other fixes that act immediately after the initial stage of time integration within a timestep (i.e. after atoms move), then the command that sets up the dynamic group should appear after those fixes. This will insure that dynamic group assignments are made after all atoms have moved.

One or more respa levels compute no forces This is computationally inefficient.

Pair COMB charge %.10f with force %.10f hit max barrier Something is possibly wrong with your model.

Pair COMB charge %.10f with force %.10f hit min barrier Something is possibly wrong with your model.

Pair brownian needs newton pair on for momentum conservation Self-explanatory.

Pair dpd needs newton pair on for momentum conservation Self-explanatory.

Pair dsmc: num_of_collisions > number_of_A Collision model in DSMC is breaking down.

Pair dsmc: num_of_collisions > number_of_B Collision model in DSMC is breaking down.

Pair style in data file differs from currently defined pair style Self-explanatory.

Pair style restartinfo set but has no restart support This pair style has a bug, where it does not support reading and writing information to a restart file, but does not set the member variable "restartinfo" to 0 as required in that case.

Particle deposition was unsuccessful The fix deposit command was not able to insert as many atoms as needed. The requested volume fraction may be too high, or other atoms may be in the insertion region.

Proc sub-domain size < neighbor skin, could lead to lost atoms The decomposition of the physical domain (likely due to load balancing) has led to a processor's sub-domain being smaller than the neighbor skin in one or more dimensions. Since reneighboring is triggered by atoms moving the skin distance, this may lead to lost atoms, if an atom moves all the way across a neighboring processor's sub-domain before reneighboring is triggered.

Reducing PPPM order b/c stencil extends beyond nearest neighbor processor This may lead to a larger grid than desired. See the kspace_modify overlap command to prevent changing of the PPPM order.

Reducing PPPMDisp Coulomb order b/c stencil extends beyond neighbor processor This may lead to a larger grid than desired. See the kspace_modify overlap command to prevent changing of the PPPM order.

Reducing PPPMDisp dispersion order b/c stencil extends beyond neighbor processor This may lead to a larger grid than desired. See the kspace_modify overlap command to prevent changing of the PPPM order.

Replacing a fix, but new group != old group The ID and style of a fix match for a fix you are changing with a fix command, but the new group you are specifying does not match the old group.

Replicating in a non-periodic dimension The parameters for a replicate command will cause a non-periodic dimension to be replicated; this may cause unwanted behavior.

Resetting reneighboring criteria during PRD A PRD simulation requires that neigh_modify settings be delay = 0, every = 1, check = yes. Since these settings were not in place, LAMMPS changed them and will restore them to their original values after the PRD simulation.

Resetting reneighboring criteria during TAD A TAD simulation requires that neigh_modify settings be delay = 0, every = 1, check = yes. Since these settings were not in place, LAMMPS changed them and will restore them to their original values after the PRD simulation.

Resetting reneighboring criteria during minimization Minimization requires that neigh_modify settings be delay = 0, every = 1, check = yes. Since these settings were not in place, LAMMPS changed them and will restore them to their original values after the minimization.

Restart file used different # of processors The restart file was written out by a LAMMPS simulation running on a different number of processors. Due to round-off, the trajectories of your restarted simulation may diverge a little more quickly than if you ran on the same # of processors.

Restart file used different 3d processor grid The restart file was written out by a LAMMPS simulation running on a different 3d grid of processors. Due to round-off, the trajectories of your restarted simulation may diverge a little more quickly than if you ran on the same # of processors.

Restart file used different boundary settings, using restart file values Your input script cannot change these restart file settings.

Restart file used different newton bond setting, using restart file value The restart file value will override the setting in the input script.

Restart file used different newton pair setting, using input script value The input script value will override the setting in the restart file.

Restrain problem: %d %ld %d %d %d %d Conformation of the 4 listed dihedral atoms is extreme; you may want to check your simulation geometry.

Running PRD with only one replica This is allowed, but you will get no parallel speed-up.

SRD bin shifting turned on due to small lamda This is done to try to preserve accuracy.

SRD bin size for fix srd differs from user request Fix SRD had to adjust the bin size to fit the simulation box. See the cubic keyword if you want this message to be an error vs warning.

SRD bins for fix srd are not cubic enough The bin shape is not within tolerance of cubic. See the cubic keyword if you want this message to be an error vs warning.

SRD particle %d started inside big particle %d on step %ld bounce %d See the inside keyword if you want this message to be an error vs warning.

SRD particle %d started inside wall %d on step %ld bounce %d See the inside keyword if you want this message to be an error vs warning.

Shake determinant < 0.0 The determinant of the quadratic equation being solved for a single cluster specified by the fix shake command is numerically suspect. LAMMPS will set it to 0.0 and continue.

Shell command '%s' failed with error '%s' Self-explanatory.

Shell command returned with non-zero status This may indicate the shell command did not operate as expected.

Should not allow rigid bodies to bounce off reflecting walls LAMMPS allows this, but their dynamics are not computed correctly.

Should not use fix nve/limit with fix shake or fix rattle This will lead to invalid constraint forces in the SHAKE/RATTLE computation.

Simulations might be very slow because of large number of structure factors Self-explanatory.

Slab correction not needed for MSM Slab correction is intended to be used with Ewald or PPPM and is not needed by MSM.

Specifying an 'subset' value of '0' is equivalent to no 'subset' keyword Self-explanatory.

System is not charge neutral, net charge = %g The total charge on all atoms on the system is not 0.0. For some KSpace solvers this is only a warning.

Table inner cutoff >= outer cutoff You specified an inner cutoff for a Coulombic table that is longer than the global cutoff. Probably not what you wanted.

Temperature for MSST is not for group all User-assigned temperature to MSST fix does not compute temperature for all atoms. Since MSST computes a global pressure, the kinetic energy contribution from the temperature is assumed to also be for all atoms. Thus the pressure used by MSST could be inaccurate.

Temperature for NPT is not for group all User-assigned temperature to NPT fix does not compute temperature for all atoms. Since NPT computes a global pressure, the kinetic energy contribution from the temperature is assumed to also be for all atoms. Thus the pressure used by NPT could be inaccurate.

Temperature for fix modify is not for group all The temperature compute is being used with a pressure calculation which does operate on group all, so this may be inconsistent.

Temperature for thermo pressure is not for group all User-assigned temperature to thermo via the thermo_modify command does not compute temperature for all atoms. Since thermo computes a global pressure, the kinetic energy contribution from the temperature is assumed to also be for all atoms. Thus the pressure printed by thermo could be inaccurate.

The fix ave/spatial command has been replaced by the more flexible fix ave/chunk and compute chunk/atom commands – fix ave/spa Self-explanatory.

The minimizer does not re-orient dipoles when using fix efield This means that only the atom coordinates will be minimized, not the orientation of the dipoles.

Too many common neighbors in CNA %d times More than the maximum # of neighbors was found multiple times. This was unexpected.

Too many inner timesteps in fix ttm Self-explanatory.

Too many neighbors in CNA for %d atoms More than the maximum # of neighbors was found multiple times. This was unexpected.

Triclinic box skew is large The displacement in a skewed direction is normally required to be less than half the box length in that dimension. E.g. the xy tilt must be between -half and +half of the x box length. You have relaxed the constraint using the box tilt command, but the warning means that a LAMMPS simulation may be inefficient as a result.

Use special bonds = 0,1,1 with bond style fene Most FENE models need this setting for the special_bonds command.

Use special bonds = 0,1,1 with bond style fene/expand Most FENE models need this setting for the special_bonds command.

Using a many-body potential with bonds/angles/dihedrals and special_bond exclusions This is likely not what you want to do. The exclusion settings will eliminate neighbors in the neighbor list, which the many-body potential needs to calculated its terms correctly.

Using compute temp/deform with inconsistent fix deform remap option Fix nvt/sllod assumes deforming atoms have a velocity profile provided by "remap v" or "remap none" as a fix deform option.

Using compute temp/deform with no fix deform defined This is probably an error, since it makes little sense to use compute temp/deform in this case.

Using fix srd with box deformation but no SRD thermostat The deformation will heat the SRD particles so this can be dangerous.

Using kspace solver on system with no charge Self-explanatory.

Using largest cut-off for lj/long/dipole/long long long Self-explanatory.

Using largest cutoff for buck/long/coul/long Self-explanatory.

Using largest cutoff for lj/long/coul/long Self-explanatory.

Using largest cutoff for pair_style lj/long/tip4p/long Self-explanatory.

Using package gpu without any pair style defined Self-explanatory.

Using pair potential shift with pair_modify compute no The shift effects will thus not be computed.

Using pair tail corrections with nonperiodic system This is probably a bogus thing to do, since tail corrections are computed by integrating the density of a periodic system out to infinity.

Using pair tail corrections with pair_modify compute no The tail corrections will thus not be computed.

pair style reax is now deprecated and will soon be retired. Users should switch to pair_style reax/c Self-explanatory.

CHAPTER

FOURTEEN

BUILDING THE LAMMPS MANUAL

Depending on how you obtained LAMMPS, the doc directory has 2 or 3 sub-directories and optionally 2 PDF files and 2 e-book format files:

```
src             # content files for LAMMPS documentation
html            # HTML version of the LAMMPS manual (see html/Manual.html)
tools           # tools and settings for building the documentation
Manual.pdf      # large PDF version of entire manual
Developer.pdf   # small PDF with info about how LAMMPS is structured
LAMMPS.epub     # Manual in ePUB e-book format
LAMMPS.mobi     # Manual in MOBI e-book format
```

If you downloaded LAMMPS as a tarball from the web site, all these directories and files should be included.

If you downloaded LAMMPS from the public git repository, then the HTML and PDF files are not included. Instead you need to create them, in one of two ways:

a. You can "fetch" the current HTML and PDF files from the LAMMPS web site. Just type "make fetch". This should download a html_www directory and Manual_www.pdf/Developer_www.pdf files. Note that if new LAMMPS features have been added more recently than the date of your LAMMPS version, the fetched documentation will include those changes (but your source code will not, unless you update your local repository).

b. You can build the HTML or PDF files yourself, by typing "make html" or "make pdf". This requires various tools including Sphinx, git, and the MathJax javascript library, which the build process will attempt to download automatically into a virtual environment in the folder doc/docenv and the folder mathjax, respectively, if not already available. This download is required only once, unless you type "make clean-all". After that, viewing and processing of the documentation can be done without internet access. To generate the PDF version of the manual, the PDFLaTeX software and several LaTeX packages are required as well. However, those cannot be installed automatically at the moment.

The generation of all documentation is managed by the Makefile in the doc directory.

```
Documentation Build Options:

make html           # generate HTML in html dir using Sphinx
make pdf            # generate 2 PDF files (Manual.pdf,Developer.pdf)
                    #   in doc dir via htmldoc and pdflatex
make fetch          # fetch HTML doc pages and 2 PDF files from web site
                    #   as a tarball and unpack into html dir and 2 PDFs
make epub           # generate LAMMPS.epub in ePUB format using Sphinx
make mobi           # generate LAMMPS.mobi in MOBI format using ebook-convert
make clean          # remove intermediate RST files created by HTML build
make clean-all      # remove entire build folder and any cached data
```

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```
make anchor_check  # check for duplicate anchor labels
make style_check   # check for complete and consistent style lists
make package_check # check for complete and consistent package lists
make spelling      # spell-check the manual
```

14.1 Installing prerequisites for HTML build

To run the HTML documentation build toolchain, Python 3 and virtualenv have to be installed. Here are instructions for common setups:

14.1.1 Ubuntu

```
sudo apt-get install python-virtualenv
```

14.1.2 Fedora (up to version 21) and Red Hat Enterprise Linux or CentOS (up to version 7.x)

```
sudo yum install python3-virtualenv
```

14.1.3 Fedora (since version 22)

```
sudo dnf install python3-virtualenv
```

14.1.4 MacOS X

Python 3

Download the latest Python 3 MacOS X package from https://www.python.org and install it. This will install both Python 3 and pip3.

virtualenv

Once Python 3 is installed, open a Terminal and type

```
pip3 install virtualenv
```

This will install virtualenv from the Python Package Index.

14.2 Installing prerequisites for epub build

14.2.1 ePUB

Same as for HTML. This uses mostly the same tools and configuration files as the HTML tree. In addition it uses LaTeX to convert embedded math expressions transparently into embedded images.

For converting the generated ePUB file to a MOBI format file (for e-book readers, like Kindle, that cannot read ePUB), you also need to have the 'ebook-convert' tool from the "calibre" software installed. http://calibre-ebook.com/ You first create the ePUB file and then convert it with 'make mobi' On the Kindle readers in particular, you also have support for PDF files, so you could download and view the PDF version as an alternative.

CHAPTER

FIFTEEN

COMMANDS

15.1 angle_coeff command

15.1.1 Syntax

```
angle_coeff N args
```

- N = angle type (see asterisk form below)
- args = coefficients for one or more angle types

15.1.2 Examples

```
angle_coeff 1 300.0 107.0
angle_coeff * 5.0
angle_coeff 2*10 5.0
```

15.1.3 Description

Specify the angle force field coefficients for one or more angle types. The number and meaning of the coefficients depends on the angle style. Angle coefficients can also be set in the data file read by the *read_data* command or in a restart file.

N can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to set the coefficients for multiple angle types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of angle types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

Note that using an *angle_coeff* command can override a previous setting for the same angle type. For example, these commands set the coeffs for all angle types, then overwrite the coeffs for just angle type 2:

```
angle_coeff * 200.0 107.0 1.2
angle_coeff 2 50.0 107.0
```

A line in a data file that specifies angle coefficients uses the exact same format as the arguments of the *angle_coeff* command in an input script, except that wild-card asterisks should not be used since coefficients for all N types must be listed in the file. For example, under the "Angle Coeffs" section of a data file, the line that corresponds to the 1st example above would be listed as

```
1 300.0 107.0
```

The *angle_style class2* is an exception to this rule, in that an additional argument is used in the input script to allow specification of the cross-term coefficients. See its doc page for details.

The list of all angle styles defined in LAMMPS is given on the *angle_style* doc page. They are also listed in more compact form on the *Commands angle* doc page.

On either of those pages, click on the style to display the formula it computes and its coefficients as specified by the associated *angle_coeff* command.

15.1.4 Restrictions

This command must come after the simulation box is defined by a *read_data*, *read_restart*, or *create_box* command.

An angle style must be defined before any angle coefficients are set, either in the input script or in a data file.

15.1.5 Related commands

angle_style

Default: none

15.2 angle_style command

15.2.1 Syntax

```
angle_style style
```

- style = *none* or *hybrid* or *charmm* or *class2* or *cosine* or *cosine/squared* or *harmonic*

15.2.2 Examples

```
angle_style harmonic
angle_style charmm
angle_style hybrid harmonic cosine
```

15.2.3 Description

Set the formula(s) LAMMPS uses to compute angle interactions between triplets of atoms, which remain in force for the duration of the simulation. The list of angle triplets is read in by a *read_data* or *read_restart* command from a data or restart file.

Hybrid models where angles are computed using different angle potentials can be setup using the *hybrid* angle style.

The coefficients associated with a angle style can be specified in a data or restart file or via the *angle_coeff* command.

All angle potentials store their coefficient data in binary restart files which means angle_style and *angle_coeff* commands do not need to be re-specified in an input script that restarts a simulation. See the *read_restart* command for details on how to do this. The one exception is that angle_style *hybrid* only stores the list of sub-styles in the restart file; angle coefficients need to be re-specified.

Note: When both an angle and pair style is defined, the *special_bonds* command often needs to be used to turn off (or weight) the pairwise interaction that would otherwise exist between 3 bonded atoms.

In the formulas listed for each angle style, *theta* is the angle between the 3 atoms in the angle.

Here is an alphabetic list of angle styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated *angle_coeff* command.

Click on the style to display the formula it computes, any additional arguments specified in the angle_style command, and coefficients specified by the associated *angle_coeff* command.

There are also additional accelerated pair styles included in the LAMMPS distribution for faster performance on CPUs, GPUs, and KNLs. The individual style names on the *Commands angle* doc page are followed by one or more of (g,i,k,o,t) to indicate which accelerated styles exist.

- *none* - turn off angle interactions
- *zero* - topology but no interactions
- *hybrid* - define multiple styles of angle interactions
- *charmm* - CHARMM angle
- *class2* - COMPASS (class 2) angle
- *class2/p6* - COMPASS (class 2) angle expanded to 6th order
- *cosine* - angle with cosine term
- *cosine/buck6d* - same as cosine with Buckingham term between 1-3 atoms
- *cosine/delta* - angle with difference of cosines
- *cosine/periodic* - DREIDING angle
- *cosine/shift* - angle cosine with a shift
- *cosine/shift/exp* - cosine with shift and exponential term in spring constant
- *cosine/squared* - angle with cosine squared term
- *cross* - cross term coupling angle and bond lengths
- *dipole* - angle that controls orientation of a point dipole
- *fourier* - angle with multiple cosine terms
- *fourier/simple* - angle with a single cosine term
- *harmonic* - harmonic angle
- *mm3* - anharmonic angle
- *quartic* - angle with cubic and quartic terms
- *sdk* - harmonic angle with repulsive SDK pair style between 1-3 atoms
- *table* - tabulated by angle

15.2.4 Restrictions

Angle styles can only be set for atom_styles that allow angles to be defined.

Most angle styles are part of the MOLECULE package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info. The doc pages for individual bond potentials tell if it is part of a package.

15.2.5 Related commands

angle_coeff

15.2.6 Default

```
angle_style none
```

15.3 atom_modify command

15.3.1 Syntax

```
atom_modify keyword values ...
```

- one or more keyword/value pairs may be appended
- keyword = *id* or *map* or *first* or *sort*

```
id value = yes or no
map value = yes or array or hash
first value = group-ID = group whose atoms will appear first in internal␣
↪atom lists
sort values = Nfreq binsize
  Nfreq = sort atoms spatially every this many time steps
  binsize = bin size for spatial sorting (distance units)
```

15.3.2 Examples

```
atom_modify map yes
atom_modify map hash sort 10000 2.0
atom_modify first colloid
```

15.3.3 Description

Modify certain attributes of atoms defined and stored within LAMMPS, in addition to what is specified by the *atom_style* command. The *id* and *map* keywords must be specified before a simulation box is defined; other keywords can be specified any time.

The *id* keyword determines whether non-zero atom IDs can be assigned to each atom. If the value is *yes*, which is the default, IDs are assigned, whether you use the *create atoms* or *read_data* or *read_restart* commands to initialize atoms. If the value is *no* the IDs for all atoms are assumed to be 0.

If atom IDs are used, they must all be positive integers. They should also be unique, though LAMMPS does not check for this. Typically they should also be consecutively numbered (from 1 to Natoms), though this is not required. Molecular *atom styles* are those that store bond topology information (styles bond, angle, molecular, full). These styles require atom IDs since the IDs are used to encode the topology. Some other LAMMPS commands also require the use of atom IDs. E.g. some many-body pair styles use them to avoid double computation of the I-J interaction between two atoms.

The only reason not to use atom IDs is if you are running an atomic simulation so large that IDs cannot be uniquely assigned. For a default LAMMPS build this limit is 2^31 or about 2 billion atoms. However, even in this case, you can use 64-bit atom IDs, allowing 2^63 or about 9e18 atoms, if you build LAMMPS with the - DLAMMPS_BIGBIG switch. This is described on the *Build_settings* doc page. If atom IDs are not used, they must be specified as 0 for all atoms, e.g. in a data or restart file.

The *map* keyword determines how atoms with specific IDs are found when required. An example are the bond (angle, etc) methods which need to find the local index of an atom with a specific global ID which is a bond (angle, etc) partner. LAMMPS performs this operation efficiently by creating a "map", which is either an *array* or *hash* table, as described below.

When the *map* keyword is not specified in your input script, LAMMPS only creates a map for *atom_styles* for molecular systems which have permanent bonds (angles, etc). No map is created for atomic systems, since it is normally not needed. However some LAMMPS commands require a map, even for atomic systems, and will generate an error if one does not exist. The *map* keyword thus allows you to force the creation of a map. The *yes* value will create either an *array* or *hash* style map, as explained in the next paragraph. The *array* and *hash* values create an atom-style or hash-style map respectively.

For an *array*-style map, each processor stores a lookup table of length N, where N is the largest atom ID in the system. This is a fast, simple method for many simulations, but requires too much memory for large simulations. For a *hash*-style map, a hash table is created on each processor, which finds an atom ID in constant time (independent of the global number of atom IDs). It can be slightly slower than the *array* map, but its memory cost is proportional to the number of atoms owned by a processor, i.e. N/P when N is the total number of atoms in the system and P is the number of processors.

The *first* keyword allows a *group* to be specified whose atoms will be maintained as the first atoms in each processor's list of owned atoms. This in only useful when the specified group is a small fraction of all the atoms, and there are other operations LAMMPS is performing that will be sped-up significantly by being able to loop over the smaller set of atoms. Otherwise the reordering required by this option will be a net slow-down. The *neigh_modify include* and *comm_modify group* commands are two examples of commands that require this setting to work efficiently. Several *fixes*, most notably time integration fixes like *fix nve*, also take advantage of this setting if the group they operate on is the group specified by this command. Note that specifying "all" as the group-ID effectively turns off the *first* option.

It is OK to use the *first* keyword with a group that has not yet been defined, e.g. to use the atom_modify first command at the beginning of your input script. LAMMPS does not use the group until a simulation is run.

The *sort* keyword turns on a spatial sorting or reordering of atoms within each processor's sub-domain every *Nfreq* timesteps. If *Nfreq* is set to 0, then sorting is turned off. Sorting can improve cache performance and thus speed-up a LAMMPS simulation, as discussed in a paper by *(Meloni)*. Its efficacy depends on the problem size (atoms/processor), how quickly the system becomes disordered, and various other factors. As a general rule, sorting is typically more

effective at speeding up simulations of liquids as opposed to solids. In tests we have done, the speed-up can range from zero to 3-4x.

Reordering is performed every *Nfreq* timesteps during a dynamics run or iterations during a minimization. More precisely, reordering occurs at the first reneighboring that occurs after the target timestep. The reordering is performed locally by each processor, using bins of the specified *binsize*. If *binsize* is set to 0.0, then a binsize equal to half the *neighbor* cutoff distance (force cutoff plus skin distance) is used, which is a reasonable value. After the atoms have been binned, they are reordered so that atoms in the same bin are adjacent to each other in the processor's 1d list of atoms.

The goal of this procedure is for atoms to put atoms close to each other in the processor's one-dimensional list of atoms that are also near to each other spatially. This can improve cache performance when pairwise interactions and neighbor lists are computed. Note that if bins are too small, there will be few atoms/bin. Likewise if bins are too large, there will be many atoms/bin. In both cases, the goal of cache locality will be undermined.

Note: Running a simulation with sorting on versus off should not change the simulation results in a statistical sense. However, a different ordering will induce round-off differences, which will lead to diverging trajectories over time when comparing two simulations. Various commands, particularly those which use random numbers (e.g. *velocity create*, and *fix langevin*), may generate (statistically identical) results which depend on the order in which atoms are processed. The order of atoms in a *dump* file will also typically change if sorting is enabled.

15.3.4 Restrictions

The *first* and *sort* options cannot be used together. Since sorting is on by default, it will be turned off if the *first* keyword is used with a group-ID that is not "all".

Related commands: none

15.3.5 Default

By default, *id* is yes. By default, atomic systems (no bond topology info) do not use a map. For molecular systems (with bond topology info), a map is used. The default map style is array if no atom ID is larger than 1 million, otherwise the default is hash. By default, a "first" group is not defined. By default, sorting is enabled with a frequency of 1000 and a binsize of 0.0, which means the neighbor cutoff will be used to set the bin size. If no neighbor cutoff is defined, sorting will be turned off.

(Meloni) Meloni, Rosati and Colombo, J Chem Phys, 126, 121102 (2007).

15.4 atom_style command

15.4.1 Syntax

```
atom_style style args
```

- style = *angle* or *atomic* or *body* or *bond* or *charge* or *dipole* or *dpd* or *edpd* or *mdpd* or *tdpd* or *electron* or *ellipsoid* or *full* or *line* or *meso* or *molecular* or *peri* or *smd* or *sphere* or *spin* or *tri* or *template* or *hybrid*

```
  args = none for any style except the following
    body args = bstyle bstyle-args
      bstyle = style of body particles
      bstyle-args = additional arguments specific to the bstyle
                    see the Howto body doc page for details
    tdpd arg = Nspecies
      Nspecies = # of chemical species
    template arg = template-ID
      template-ID = ID of molecule template specified in a separate␣
↪molecule command
    hybrid args = list of one or more sub-styles, each with their args
```

- accelerated styles (with same args) = *angle/kk* or *atomic/kk* or *bond/kk* or *charge/kk* or *full/kk* or *molecular/kk*

15.4.2 Examples

```
atom_style atomic
atom_style bond
atom_style full
atom_style body nparticle 2 10
atom_style hybrid charge bond
atom_style hybrid charge body nparticle 2 5
atom_style spin
atom_style template myMols
atom_style tdpd 2
```

15.4.3 Description

Define what style of atoms to use in a simulation. This determines what attributes are associated with the atoms. This command must be used before a simulation is setup via a *read_data*, *read_restart*, or *create_box* command.

Note: Many of the atom styles discussed here are only enabled if LAMMPS was built with a specific package, as listed below in the Restrictions section.

Once a style is assigned, it cannot be changed, so use a style general enough to encompass all attributes. E.g. with style *bond*, angular terms cannot be used or added later to the model. It is OK to use a style more general than needed, though it may be slightly inefficient.

The choice of style affects what quantities are stored by each atom, what quantities are communicated between processors to enable forces to be computed, and what quantities are listed in the data file read by the *read_data* command.

These are the additional attributes of each style and the typical kinds of physical systems they are used to model. All styles store coordinates, velocities, atom IDs and types. See the *read_data*, *create_atoms*, and *set* commands for info on how to set these various quantities.

angle	bonds and angles	bead-spring polymers with stiffness
atomic	only the default values	coarse-grain liquids, solids, metals
body	mass, inertia moments, quaternion, angular momentum	arbitrary bodies
bond	bonds	bead-spring polymers
charge	charge	atomic system with charges
dipole	charge and dipole moment	system with dipolar particles
dpd	internal temperature and internal energies	DPD particles
edpd	temperature and heat capacity	eDPD particles
mdpd	density	mDPD particles
tdpd	chemical concentration	tDPD particles
electron	charge and spin and eradius	electronic force field
ellipsoid	shape, quaternion, angular momentum	aspherical particles
full	molecular + charge	bio-molecules
line	end points, angular velocity	rigid bodies
meso	rho, e, cv	SPH particles
molecular	bonds, angles, dihedrals, impropers	uncharged molecules
peri	mass, volume	mesoscopic Peridynamic models
smd	volume, kernel diameter, contact radius, mass	solid and fluid SPH particles
sphere	diameter, mass, angular velocity	granular models
spin	magnetic moment	system with magnetic particles
template	template index, template atom	small molecules with fixed topology
tri	corner points, angular momentum	rigid bodies
wavepacket	charge, spin, eradius, etag, cs_re, cs_im	AWPMD

Note: It is possible to add some attributes, such as a molecule ID, to atom styles that do not have them via the *fix property/atom* command. This command also allows new custom attributes consisting of extra integer or floating-point values to be added to atoms. See the *fix property/atom* doc page for examples of cases where this is useful and details on how to initialize, access, and output the custom values.

All of the above styles define point particles, except the *sphere*, *ellipsoid*, *electron*, *peri*, *wavepacket*, *line*, *tri*, and *body* styles, which define finite-size particles. See the *Howto spherical* doc page for an overview of using finite-size particle models with LAMMPS.

All of the point-particle styles assign mass to particles on a per-type basis, using the *mass* command, The finite-size particle styles assign mass to individual particles on a per-particle basis.

For the *sphere* style, the particles are spheres and each stores a per-particle diameter and mass. If the diameter > 0.0, the particle is a finite-size sphere. If the diameter = 0.0, it is a point particle. Note that by use of the *disc* keyword with the *fix nve/sphere*, *fix nvt/sphere*, *fix nph/sphere*, *fix npt/sphere* commands, spheres can be effectively treated as 2d discs for a 2d simulation if desired. See also the *set density/disc* command.

For the *ellipsoid* style, the particles are ellipsoids and each stores a flag which indicates whether it is a finite-size ellipsoid or a point particle. If it is an ellipsoid, it also stores a shape vector with the 3 diameters of the ellipsoid and a quaternion 4-vector with its orientation.

For the *dipole* style, a point dipole is defined for each point particle. Note that if you wish the particles to be finite-size spheres as in a Stockmayer potential for a dipolar fluid, so that the particles can rotate due to dipole-dipole interactions, then you need to use atom_style hybrid sphere dipole, which will assign both a diameter and dipole moment to each particle.

For the *electron* style, the particles representing electrons are 3d Gaussians with a specified position and bandwidth or uncertainty in position, which is represented by the eradius = electron size.

For the *peri* style, the particles are spherical and each stores a per-particle mass and volume.

The *dpd* style is for dissipative particle dynamics (DPD) particles. Note that it is part of the USER-DPD package, and is not for use with the *pair_style dpd or dpd/stat* commands, which can simply use atom_style atomic. Atom_style dpd extends DPD particle properties with internal temperature (dpdTheta), internal conductive energy (uCond), internal mechanical energy (uMech), and internal chemical energy (uChem).

The *edpd* style is for energy-conserving dissipative particle dynamics (eDPD) particles which store a temperature (edpd_temp), and heat capacity(edpd_cv).

The *mdpd* style is for many-body dissipative particle dynamics (mDPD) particles which store a density (rho) for considering density-dependent many-body interactions.

The *tdpd* style is for transport dissipative particle dynamics (tDPD) particles which store a set of chemical concentration. An integer "cc_species" is required to specify the number of chemical species involved in a tDPD system.

The *meso* style is for smoothed particle hydrodynamics (SPH) particles which store a density (rho), energy (e), and heat capacity (cv).

The *smd* style is for a general formulation of Smooth Particle Hydrodynamics. Both fluids and solids can be modeled. Particles store the mass and volume of an integration point, a kernel diameter used for calculating the field variables (e.g. stress and deformation) and a contact radius for calculating repulsive forces which prevent individual physical bodies from penetrating each other.

For the *spin* style, a magnetic spin is associated to each atom. Those spins have a norm (their magnetic moment) and a direction.

The *wavepacket* style is similar to *electron*, but the electrons may consist of several Gaussian wave packets, summed up with coefficients cs= (cs_re,cs_im). Each of the wave packets is treated as a separate particle in LAMMPS, wave packets belonging to the same electron must have identical *etag* values.

For the *line* style, the particles are idealized line segments and each stores a per-particle mass and length and orientation (i.e. the end points of the line segment).

For the *tri* style, the particles are planar triangles and each stores a per-particle mass and size and orientation (i.e. the corner points of the triangle).

The *template* style allows molecular topology (bonds,angles,etc) to be defined via a molecule template using the *molecule* command. The template stores one or more molecules with a single copy of the topology info (bonds,angles,etc) of each. Individual atoms only store a template index and template atom to identify which molecule and which atom-within-the-molecule they represent. Using the *template* style instead of the *bond*, *angle*, *molecular* styles can save memory for systems comprised of a large number of small molecules, all of a single type (or small number of types). See the paper by Grime and Voth, in *(Grime)*, for examples of how this can be advantageous for large-scale coarse-grained systems.

Note: When using the *template* style with a *molecule template* that contains multiple molecules, you should insure the atom types, bond types, angle_types, etc in all the molecules are consistent. E.g. if one molecule represents H2O and another CO2, then you probably do not want each molecule file to define 2 atom types and a single bond type, because they will conflict with each other when a mixture system of H2O and CO2 molecules is defined, e.g. by the *read_data* command. Rather the H2O molecule should define atom types 1 and 2, and bond type 1. And the CO2 molecule should define atom types 3 and 4 (or atom types 3 and 2 if a single oxygen type is desired), and bond type 2.

For the *body* style, the particles are arbitrary bodies with internal attributes defined by the "style" of the bodies, which is specified by the *bstyle* argument. Body particles can represent complex entities, such as surface meshes of discrete points, collections of sub-particles, deformable objects, etc.

The *Howto body* doc page describes the body styles LAMMPS currently supports, and provides more details as to the kind of body particles they represent. For all styles, each body particle stores moments of inertia and a quaternion 4-vector, so that its orientation and position can be time integrated due to forces and torques.

Note that there may be additional arguments required along with the *bstyle* specification, in the atom_style body command. These arguments are described on the *Howto body* doc page.

Typically, simulations require only a single (non-hybrid) atom style. If some atoms in the simulation do not have all the properties defined by a particular style, use the simplest style that defines all the needed properties by any atom. For example, if some atoms in a simulation are charged, but others are not, use the *charge* style. If some atoms have bonds, but others do not, use the *bond* style.

The only scenario where the *hybrid* style is needed is if there is no single style which defines all needed properties of all atoms. For example, as mentioned above, if you want dipolar particles which will rotate due to torque, you need to use "atom_style hybrid sphere dipole". When a hybrid style is used, atoms store and communicate the union of all quantities implied by the individual styles.

When using the *hybrid* style, you cannot combine the *template* style with another molecular style that stores bond,angle,etc info on a per-atom basis.

LAMMPS can be extended with new atom styles as well as new body styles; see the *Modify* doc page.

Styles with a *kk* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

Note that other acceleration packages in LAMMPS, specifically the GPU, USER-INTEL, USER-OMP, and OPT packages do not use accelerated atom styles.

The accelerated styles are part of the KOKKOS package. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

15.4.4 Restrictions

This command cannot be used after the simulation box is defined by a *read_data* or *create_box* command.

Many of the styles listed above are only enabled if LAMMPS was built with a specific package, as listed below. See the *Build package* doc page for more info.

The *angle*, *bond*, *full*, *molecular*, and *template* styles are part of the MOLECULE package.

The *line* and *tri* styles are part of the ASPHERE package.

The *body* style is part of the BODY package.

The *dipole* style is part of the DIPOLE package.

The *peri* style is part of the PERI package for Peridynamics.

The *electron* style is part of the USER-EFF package for *electronic force fields*.

The *dpd* style is part of the USER-DPD package for dissipative particle dynamics (DPD).

The *edpd*, *mdpd*, and *tdpd* styles are part of the USER-MESO package for energy-conserving dissipative particle dynamics (eDPD), many-body dissipative particle dynamics (mDPD), and transport dissipative particle dynamics (tDPD), respectively.

The *meso* style is part of the USER-SPH package for smoothed particle hydrodynamics (SPH). See this PDF guide to using SPH in LAMMPS.

The *spin* style is part of the SPIN package.

The *wavepacket* style is part of the USER-AWPMD package for the *antisymmetrized wave packet MD method*.

15.4.5 Related commands

read_data, *pair_style*

15.4.6 Default

atom_style atomic

(Grime) Grime and Voth, to appear in J Chem Theory & Computation (2014).

15.5 balance command

15.5.1 Syntax

```
balance thresh style args ... keyword args ...
```

- thresh = imbalance threshold that must be exceeded to perform a re-balance
- one style/arg pair can be used (or multiple for *x*,*y*,*z*)
- style = *x* or *y* or *z* or *shift* or *rcb*

```
x args = uniform or Px-1 numbers between 0 and 1
  uniform = evenly spaced cuts between processors in x dimension
  numbers = Px-1 ascending values between 0 and 1, Px - # of processors␣
↪in x dimension
  x can be specified together with y or z
y args = uniform or Py-1 numbers between 0 and 1
  uniform = evenly spaced cuts between processors in y dimension
  numbers = Py-1 ascending values between 0 and 1, Py - # of processors␣
↪in y dimension
  y can be specified together with x or z
z args = uniform or Pz-1 numbers between 0 and 1
  uniform = evenly spaced cuts between processors in z dimension
  numbers = Pz-1 ascending values between 0 and 1, Pz - # of processors␣
↪in z dimension
  z can be specified together with x or y
shift args = dimstr Niter stopthresh
  dimstr = sequence of letters containing "x" or "y" or "z", each not␣
↪more than once
  Niter = # of times to iterate within each dimension of dimstr sequence
  stopthresh = stop balancing when this imbalance threshold is reached
rcb args = none
```

- zero or more keyword/arg pairs may be appended

- keyword = *weight* or *out*

```
weight style args = use weighted particle counts for the balancing
  style = group or neigh or time or var or store
    group args = Ngroup group1 weight1 group2 weight2 ...
      Ngroup = number of groups with assigned weights
      group1, group2, ... = group IDs
      weight1, weight2, ...   = corresponding weight factors
    neigh factor = compute weight based on number of neighbors
      factor = scaling factor (> 0)
    time factor = compute weight based on time spend computing
      factor = scaling factor (> 0)
    var name = take weight from atom-style variable
      name = name of the atom-style variable
    store name = store weight in custom atom property defined by fix␣
↪property/atom command
      name = atom property name (without d_ prefix)
out arg = filename
  filename = write each processor's sub-domain to a file
```

15.5.2 Examples

```
balance 0.9 x uniform y 0.4 0.5 0.6
balance 1.2 shift xz 5 1.1
balance 1.0 shift xz 5 1.1
balance 1.1 rcb
balance 1.0 shift x 10 1.1 weight group 2 fast 0.5 slow 2.0
balance 1.0 shift x 10 1.1 weight time 0.8 weight neigh 0.5 weight store balance
balance 1.0 shift x 20 1.0 out tmp.balance
```

15.5.3 Description

This command adjusts the size and shape of processor sub-domains within the simulation box, to attempt to balance the number of atoms or particles and thus indirectly the computational cost (load) more evenly across processors. The load balancing is "static" in the sense that this command performs the balancing once, before or between simulations. The processor sub-domains will then remain static during the subsequent run. To perform "dynamic" balancing, see the *fix balance* command, which can adjust processor sub-domain sizes and shapes on-the-fly during a *run*.

Load-balancing is typically most useful if the particles in the simulation box have a spatially-varying density distribution or when the computational cost varies significantly between different particles. E.g. a model of a vapor/liquid interface, or a solid with an irregular-shaped geometry containing void regions, or *hybrid pair style simulations* which combine pair styles with different computational cost. In these cases, the LAMMPS default of dividing the simulation box volume into a regular-spaced grid of 3d bricks, with one equal-volume sub-domain per processor, may assign numbers of particles per processor in a way that the computational effort varies significantly. This can lead to poor performance when the simulation is run in parallel.

The balancing can be performed with or without per-particle weighting. With no weighting, the balancing attempts to assign an equal number of particles to each processor. With weighting, the balancing attempts to assign an equal aggregate computational weight to each processor, which typically induces a different number of atoms assigned to each processor. Details on the various weighting options and examples for how they can be used are *given below*.

Note that the *processors* command allows some control over how the box volume is split across processors. Specifically, for a Px by Py by Pz grid of processors, it allows choice of Px, Py, and Pz, subject to the constraint that Px * Py

* Pz = P, the total number of processors. This is sufficient to achieve good load-balance for some problems on some processor counts. However, all the processor sub-domains will still have the same shape and same volume.

The requested load-balancing operation is only performed if the current "imbalance factor" in particles owned by each processor exceeds the specified *thresh* parameter. The imbalance factor is defined as the maximum number of particles (or weight) owned by any processor, divided by the average number of particles (or weight) per processor. Thus an imbalance factor of 1.0 is perfect balance.

As an example, for 10000 particles running on 10 processors, if the most heavily loaded processor has 1200 particles, then the factor is 1.2, meaning there is a 20% imbalance. Note that a re-balance can be forced even if the current balance is perfect (1.0) be specifying a *thresh* < 1.0.

Note: Balancing is performed even if the imbalance factor does not exceed the *thresh* parameter if a "grid" style is specified when the current partitioning is "tiled". The meaning of "grid" vs "tiled" is explained below. This is to allow forcing of the partitioning to "grid" so that the *comm_style brick* command can then be used to replace a current *comm_style tiled* setting.

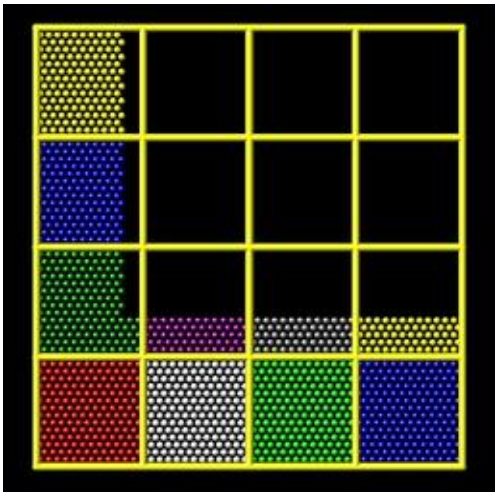
When the balance command completes, it prints statistics about the result, including the change in the imbalance factor and the change in the maximum number of particles on any processor. For "grid" methods (defined below) that create a logical 3d grid of processors, the positions of all cutting planes in each of the 3 dimensions (as fractions of the box length) are also printed.

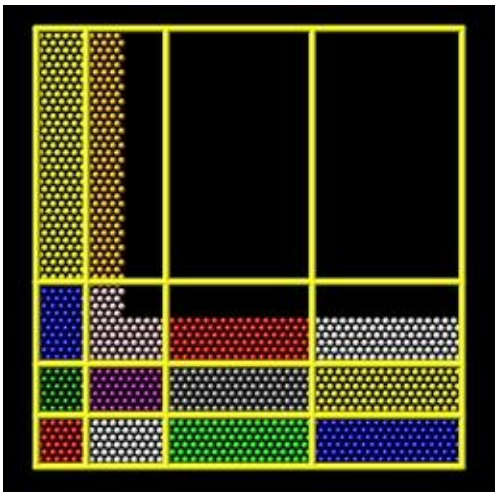
Note: This command attempts to minimize the imbalance factor, as defined above. But depending on the method a perfect balance (1.0) may not be achieved. For example, "grid" methods (defined below) that create a logical 3d grid cannot achieve perfect balance for many irregular distributions of particles. Likewise, if a portion of the system is a perfect lattice, e.g. the initial system is generated by the *create_atoms* command, then "grid" methods may be unable to achieve exact balance. This is because entire lattice planes will be owned or not owned by a single processor.

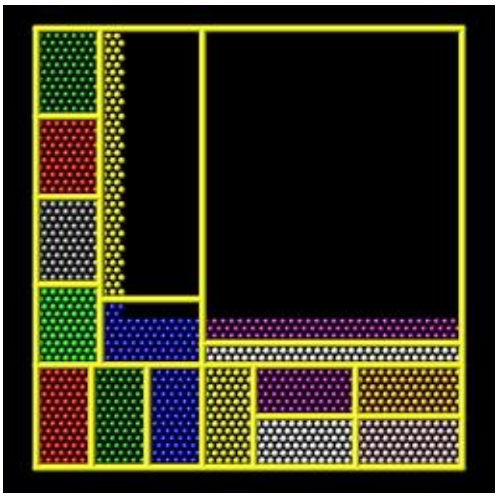
Note: The imbalance factor is also an estimate of the maximum speed-up you can hope to achieve by running a perfectly balanced simulation versus an imbalanced one. In the example above, the 10000 particle simulation could run up to 20% faster if it were perfectly balanced, versus when imbalanced. However, computational cost is not strictly proportional to particle count, and changing the relative size and shape of processor sub-domains may lead to additional computational and communication overheads, e.g. in the PPPM solver used via the *kspace_style* command. Thus you should benchmark the run times of a simulation before and after balancing.

The method used to perform a load balance is specified by one of the listed styles (or more in the case of *x*,*y*,*z*), which are described in detail below. There are 2 kinds of styles.

The *x*, *y*, *z*, and *shift* styles are "grid" methods which produce a logical 3d grid of processors. They operate by changing the cutting planes (or lines) between processors in 3d (or 2d), to adjust the volume (area in 2d) assigned to each processor, as in the following 2d diagram where processor sub-domains are shown and particles are colored by the processor that owns them. The leftmost diagram is the default partitioning of the simulation box across processors (one sub-box for each of 16 processors); the middle diagram is after a "grid" method has been applied.







The *rcb* style is a "tiling" method which does not produce a logical 3d grid of processors. Rather it tiles the simulation domain with rectangular sub-boxes of varying size and shape in an irregular fashion so as to have equal numbers of particles (or weight) in each sub-box, as in the rightmost diagram above.

The "grid" methods can be used with either of the *comm_style* command options, *brick* or *tiled*. The "tiling" methods can only be used with *comm_style tiled*. Note that it can be useful to use a "grid" method with *comm_style tiled* to return the domain partitioning to a logical 3d grid of processors so that "comm_style brick" can afterwords be specified

for subsequent *run* commands.

When a "grid" method is specified, the current domain partitioning can be either a logical 3d grid or a tiled partitioning. In the former case, the current logical 3d grid is used as a starting point and changes are made to improve the imbalance factor. In the latter case, the tiled partitioning is discarded and a logical 3d grid is created with uniform spacing in all dimensions. This becomes the starting point for the balancing operation.

When a "tiling" method is specified, the current domain partitioning ("grid" or "tiled") is ignored, and a new partitioning is computed from scratch.

The *x*, *y*, and *z* styles invoke a "grid" method for balancing, as described above. Note that any or all of these 3 styles can be specified together, one after the other, but they cannot be used with any other style. This style adjusts the position of cutting planes between processor sub-domains in specific dimensions. Only the specified dimensions are altered.

The *uniform* argument spaces the planes evenly, as in the left diagrams above. The *numeric* argument requires listing Ps-1 numbers that specify the position of the cutting planes. This requires knowing Ps = Px or Py or Pz = the number of processors assigned by LAMMPS to the relevant dimension. This assignment is made (and the Px, Py, Pz values printed out) when the simulation box is created by the "create_box" or "read_data" or "read_restart" command and is influenced by the settings of the *processors* command.

Each of the numeric values must be between 0 and 1, and they must be listed in ascending order. They represent the fractional position of the cutting place. The left (or lower) edge of the box is 0.0, and the right (or upper) edge is 1.0. Neither of these values is specified. Only the interior Ps-1 positions are specified. Thus is there are 2 processors in the x dimension, you specify a single value such as 0.75, which would make the left processor's sub-domain 3x larger than the right processor's sub-domain.

The *shift* style invokes a "grid" method for balancing, as described above. It changes the positions of cutting planes between processors in an iterative fashion, seeking to reduce the imbalance factor, similar to how the *fix balance shift* command operates.

The *dimstr* argument is a string of characters, each of which must be an "x" or "y" or "z". Eacn character can appear zero or one time, since there is no advantage to balancing on a dimension more than once. You should normally only list dimensions where you expect there to be a density variation in the particles.

Balancing proceeds by adjusting the cutting planes in each of the dimensions listed in *dimstr*, one dimension at a time. For a single dimension, the balancing operation (described below) is iterated on up to *Niter* times. After each dimension finishes, the imbalance factor is re-computed, and the balancing operation halts if the *stopthresh* criterion is met.

A re-balance operation in a single dimension is performed using a recursive multisectioning algorithm, where the position of each cutting plane (line in 2d) in the dimension is adjusted independently. This is similar to a recursive bisectioning for a single value, except that the bounds used for each bisectioning take advantage of information from neighboring cuts if possible. At each iteration, the count of particles on either side of each plane is tallied. If the counts do not match the target value for the plane, the position of the cut is adjusted to be halfway between a low and high bound. The low and high bounds are adjusted on each iteration, using new count information, so that they become closer together over time. Thus as the recursion progresses, the count of particles on either side of the plane gets closer to the target value.

Once the re-balancing is complete and final processor sub-domains assigned, particles are migrated to their new owning processor, and the balance procedure ends.

Note: At each re-balance operation, the bisectioning for each cutting plane (line in 2d) typically starts with low and high bounds separated by the extent of a processor's sub-domain in one dimension. The size of this bracketing region shrinks by 1/2 every iteration. Thus if *Niter* is specified as 10, the cutting plane will typically be positioned to 1 part

in 1000 accuracy (relative to the perfect target position). For *Niter* = 20, it will be accurate to 1 part in a million. Thus there is no need ot set *Niter* to a large value. LAMMPS will check if the threshold accuracy is reached (in a dimension) is less iterations than *Niter* and exit early. However, *Niter* should also not be set too small, since it will take roughly the same number of iterations to converge even if the cutting plane is initially close to the target value.

The *rcb* style invokes a "tiled" method for balancing, as described above. It performs a recursive coordinate bisectioning (RCB) of the simulation domain. The basic idea is as follows.

The simulation domain is cut into 2 boxes by an axis-aligned cut in one of the dimensions, leaving one new sub-box on either side of the cut. Which dimension is chosen for the cut depends on the particle (weight) distribution within the parent box. Normally the longest dimension of the box is cut, but if all (or most) of the particles are at one end of the box, a cut may be performed in another dimension to induce sub-boxes that are more cube-ish (3d) or square-ish (2d) in shape.

After the cut is made, all the processors are also partitioned into 2 groups, half assigned to the box on the lower side of the cut, and half to the box on the upper side. (If the processor count is odd, one side gets an extra processor.) The cut is positioned so that the number of (weighted) particles in the lower box is exactly the number that the processors assigned to that box should own for load balance to be perfect. This also makes load balance for the upper box perfect. The positioning of the cut is done iteratively, by a bisectioning method (median search). Note that counting particles on either side of the cut requires communication between all processors at each iteration.

That is the procedure for the first cut. Subsequent cuts are made recursively, in exactly the same manner. The subset of processors assigned to each box make a new cut in one dimension of that box, splitting the box, the subset of processors, and the particles in the box in two. The recursion continues until every processor is assigned a sub-box of the entire simulation domain, and owns the (weighted) particles in that sub-box.

This sub-section describes how to perform weighted load balancing using the *weight* keyword.

By default, all particles have a weight of 1.0, which means each particle is assumed to require the same amount of computation during a timestep. There are, however, scenarios where this is not a good assumption. Measuring the computational cost for each particle accurately would be impractical and slow down the computation. Instead the *weight* keyword implements several ways to influence the per-particle weights empirically by properties readily available or using the user's knowledge of the system. Note that the absolute value of the weights are not important; only their relative ratios affect which particle is assigned to which processor. A particle with a weight of 2.5 is assumed to require 5x more computational than a particle with a weight of 0.5. For all the options below the weight assigned to a particle must be a positive value; an error will be be generated if a weight is <= 0.0.

Below is a list of possible weight options with a short description of their usage and some example scenarios where they might be applicable. It is possible to apply multiple weight flags and the weightings they induce will be combined through multiplication. Most of the time, however, it is sufficient to use just one method.

The *group* weight style assigns weight factors to specified *groups* of particles. The *group* style keyword is followed by the number of groups, then pairs of group IDs and the corresponding weight factor. If a particle belongs to none of the specified groups, its weight is not changed. If it belongs to multiple groups, its weight is the product of the weight factors.

This weight style is useful in combination with pair style *hybrid*, e.g. when combining a more costly many-body potential with a fast pair-wise potential. It is also useful when using *run_style respa* where some portions of the system have many bonded interactions and others none. It assumes that the computational cost for each group remains constant over time. This is a purely empirical weighting, so a series test runs to tune the assigned weight factors for optimal performance is recommended.

The *neigh* weight style assigns the same weight to each particle owned by a processor based on the total count of neighbors in the neighbor list owned by that processor. The motivation is that more neighbors means a higher computational cost. The style does not use neighbors per atom to assign a unique weight to each atom, because that value can vary depending on how the neighbor list is built.

The *factor* setting is applied as an overall scale factor to the *neigh* weights which allows adjustment of their impact on the balancing operation. The specified *factor* value must be positive. A value > 1.0 will increase the weights so that the ratio of max weight to min weight increases by *factor*. A value < 1.0 will decrease the weights so that the ratio of max weight to min weight decreases by *factor*. In both cases the intermediate weight values increase/decrease proportionally as well. A value = 1.0 has no effect on the *neigh* weights. As a rule of thumb, we have found a *factor* of about 0.8 often results in the best performance, since the number of neighbors is likely to overestimate the ideal weight.

This weight style is useful for systems where there are different cutoffs used for different pairs of interactions, or the density fluctuates, or a large number of particles are in the vicinity of a wall, or a combination of these effects. If a simulation uses multiple neighbor lists, this weight style will use the first suitable neighbor list it finds. It will not request or compute a new list. A warning will be issued if there is no suitable neighbor list available or if it is not current, e.g. if the balance command is used before a *run* or *minimize* command is used, in which case the neighbor list may not yet have been built. In this case no weights are computed. Inserting a *run 0 post no* command before issuing the *balance* command, may be a workaround for this case, as it will induce the neighbor list to be built.

The *time* weight style uses *timer data* to estimate weights. It assigns the same weight to each particle owned by a processor based on the total computational time spent by that processor. See details below on what time window is used. It uses the same timing information as is used for the *MPI task timing breakdown*, namely, for sections *Pair*, *Bond*, *Kspace*, and *Neigh*. The time spent in those portions of the timestep are measured for each MPI rank, summed, then divided by the number of particles owned by that processor. I.e. the weight is an effective CPU time/particle averaged over the particles on that processor.

The *factor* setting is applied as an overall scale factor to the *time* weights which allows adjustment of their impact on the balancing operation. The specified *factor* value must be positive. A value > 1.0 will increase the weights so that the ratio of max weight to min weight increases by *factor*. A value < 1.0 will decrease the weights so that the ratio of max weight to min weight decreases by *factor*. In both cases the intermediate weight values increase/decrease proportionally as well. A value = 1.0 has no effect on the *time* weights. As a rule of thumb, effective values to use are typically between 0.5 and 1.2. Note that the timer quantities mentioned above can be affected by communication which occurs in the middle of the operations, e.g. pair styles with intermediate exchange of data witin the force computation, and likewise for KSpace solves.

When using the *time* weight style with the *balance* command, the timing data is taken from the preceding run command, i.e. the timings are for the entire previous run. For the *fix balance* command the timing data is for only the timesteps since the last balancing operation was performed. If timing information for the required sections is not available, e.g. at the beginning of a run, or when the *timer* command is set to either *loop* or *off*, a warning is issued. In this case no weights are computed.

Note: The *time* weight style is the most generic option, and should be tried first, unless the *group* style is easily applicable. However, since the computed cost function is averaged over all particles on a processor, the weights may not be highly accurate. This style can also be effective as a secondary weight in combination with either *group* or *neigh* to offset some of inaccuracies in either of those heuristics.

The *var* weight style assigns per-particle weights by evaluating an *atom-style variable* specified by *name*. This is provided as a more flexible alternative to the *group* weight style, allowing definition of a more complex heuristics based on information (global and per atom) available inside of LAMMPS. For example, atom-style variables can reference the position of a particle, its velocity, the volume of its Voronoi cell, etc.

The *store* weight style does not compute a weight factor. Instead it stores the current accumulated weights in a custom per-atom property specified by *name*. This must be a property defined as *d_name* via the *fix property/atom* command. Note that these custom per-atom properties can be output in a *dump* file, so this is a way to examine, debug, or visualize the per-particle weights computed during the load-balancing operation.

The *out* keyword writes a text file to the specified *filename* with the results of the balancing operation. The file contains the bounds of the sub-domain for each processor after the balancing operation completes. The format of the file is

compatible with the Pizza.py *mdump* tool which has support for manipulating and visualizing mesh files. An example is shown here for a balancing by 4 processors for a 2d problem:

```
ITEM: TIMESTEP
0
ITEM: NUMBER OF NODES
16
ITEM: BOX BOUNDS
0 10
0 10
0 10
ITEM: NODES
1 1 0 0 0
2 1 5 0 0
3 1 5 5 0
4 1 0 5 0
5 1 5 0 0
6 1 10 0 0
7 1 10 5 0
8 1 5 5 0
9 1 0 5 0
10 1 5 5 0
11 1 5 10 0
12 1 10 5 0
13 1 5 5 0
14 1 10 5 0
15 1 10 10 0
16 1 5 10 0
ITEM: TIMESTEP
0
ITEM: NUMBER OF SQUARES
4
ITEM: SQUARES
1 1 1 2 3 4
2 1 5 6 7 8
3 1 9 10 11 12
4 1 13 14 15 16
```

The coordinates of all the vertices are listed in the NODES section, 5 per processor. Note that the 4 sub-domains share vertices, so there will be duplicate nodes in the list.

The "SQUARES" section lists the node IDs of the 4 vertices in a rectangle for each processor (1 to 4).

For a 3d problem, the syntax is similar with 8 vertices listed for each processor, instead of 4, and "SQUARES" replaced by "CUBES".

15.5.4 Restrictions

For 2d simulations, the *z* style cannot be used. Nor can a "z" appear in *dimstr* for the *shift* style.

Balancing through recursive bisectioning (*rcb* style) requires *comm_style tiled*

15.5.5 Related commands

group, *processors*, *fix balance*, *comm_style*

Default: none

15.6 bond_coeff command

15.6.1 Syntax

```
bond_coeff N args
```

- N = bond type (see asterisk form below)
- args = coefficients for one or more bond types

15.6.2 Examples

```
bond_coeff 5 80.0 1.2
bond_coeff * 30.0 1.5 1.0 1.0
bond_coeff 1*4 30.0 1.5 1.0 1.0
bond_coeff 1 harmonic 200.0 1.0
```

15.6.3 Description

Specify the bond force field coefficients for one or more bond types. The number and meaning of the coefficients depends on the bond style. Bond coefficients can also be set in the data file read by the *read_data* command or in a restart file.

N can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to set the coefficients for multiple bond types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of bond types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

Note that using a bond_coeff command can override a previous setting for the same bond type. For example, these commands set the coeffs for all bond types, then overwrite the coeffs for just bond type 2:

```
bond_coeff * 100.0 1.2
bond_coeff 2 200.0 1.2
```

A line in a data file that specifies bond coefficients uses the exact same format as the arguments of the bond_coeff command in an input script, except that wild-card asterisks should not be used since coefficients for all N types must be listed in the file. For example, under the "Bond Coeffs" section of a data file, the line that corresponds to the 1st example above would be listed as

```
5 80.0 1.2
```

The list of all bond styles defined in LAMMPS is given on the *bond_style* doc page. They are also listed in more compact form on the *Commands bond* doc page.

On either of those pages, click on the style to display the formula it computes and its coefficients as specified by the associated bond_coeff command.

15.6.4 Restrictions

This command must come after the simulation box is defined by a *read_data*, *read_restart*, or *create_box* command.

A bond style must be defined before any bond coefficients are set, either in the input script or in a data file.

15.6.5 Related commands

bond_style

Default: none

15.7 bond_style command

15.7.1 Syntax

```
bond_style style args
```

- style = *none* or *hybrid* or *class2* or *fene* or *fene/expand* or *harmonic* or *morse* or *nonlinear* or *quartic*
- args = none for any style except *hybrid*
  - *hybrid* args = list of one or more styles

15.7.2 Examples

```
bond_style harmonic
bond_style fene
bond_style hybrid harmonic fene
```

15.7.3 Description

Set the formula(s) LAMMPS uses to compute bond interactions between pairs of atoms. In LAMMPS, a bond differs from a pairwise interaction, which are set via the *pair_style* command. Bonds are defined between specified pairs of atoms and remain in force for the duration of the simulation (unless the bond breaks which is possible in some bond potentials). The list of bonded atoms is read in by a *read_data* or *read_restart* command from a data or restart file. By contrast, pair potentials are typically defined between all pairs of atoms within a cutoff distance and the set of active interactions changes over time.

Hybrid models where bonds are computed using different bond potentials can be setup using the *hybrid* bond style.

The coefficients associated with a bond style can be specified in a data or restart file or via the *bond_coeff* command.

All bond potentials store their coefficient data in binary restart files which means bond_style and *bond_coeff* commands do not need to be re-specified in an input script that restarts a simulation. See the *read_restart* command for details on how to do this. The one exception is that bond_style *hybrid* only stores the list of sub-styles in the restart file; bond coefficients need to be re-specified.

Note: When both a bond and pair style is defined, the *special_bonds* command often needs to be used to turn off (or weight) the pairwise interaction that would otherwise exist between 2 bonded atoms.

In the formulas listed for each bond style, *r* is the distance between the 2 atoms in the bond.

Here is an alphabetic list of bond styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated *bond_coeff* command.

Click on the style to display the formula it computes, any additional arguments specified in the bond_style command, and coefficients specified by the associated *bond_coeff* command.

There are also additional accelerated pair styles included in the LAMMPS distribution for faster performance on CPUs, GPUs, and KNLs. The individual style names on the *Commands bond* doc page are followed by one or more of (g,i,k,o,t) to indicate which accelerated styles exist.

- *none* - turn off bonded interactions
- *zero* - topology but no interactions
- *hybrid* - define multiple styles of bond interactions
- *class2* - COMPASS (class 2) bond
- *fene* - FENE (finite-extensible non-linear elastic) bond
- *fene/expand* - FENE bonds with variable size particles
- *gromos* - GROMOS force field bond
- *harmonic* - harmonic bond
- *harmonic/shift* - shifted harmonic bond
- *harmonic/shift/cut* - shifted harmonic bond with a cutoff
- *mm3* - MM3 anharmonic bond
- *morse* - Morse bond
- *nonlinear* - nonlinear bond
- *oxdna/fene* - modified FENE bond suitable for DNA modeling
- *oxdna2/fene* - same as oxdna but used with different pair styles
- *oxrna2/fene* - modified FENE bond suitable for RNA modeling
- *quartic* - breakable quartic bond
- *table* - tabulated by bond length

15.7.4 Restrictions

Bond styles can only be set for atom styles that allow bonds to be defined.

Most bond styles are part of the MOLECULE package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info. The doc pages for individual bond potentials tell if it is part of a package.

15.7.5 Related commands

bond_coeff, *delete_bonds*

15.7.6 Default

```
bond_style none
```

15.8 bond_write command

15.8.1 Syntax

```
bond_write btype N inner outer file keyword itype jtype
```

- btype = bond types
- N = # of values
- inner,outer = inner and outer bond length (distance units)
- file = name of file to write values to
- keyword = section name in file for this set of tabulated values
- itype,jtype = 2 atom types (optional)

15.8.2 Examples

```
bond_write 1 500 0.5 3.5 table.txt Harmonic_1
bond_write 3 1000 0.1 6.0 table.txt Morse
```

15.8.3 Description

Write energy and force values to a file as a function of distance for the currently defined bond potential. This is useful for plotting the potential function or otherwise debugging its values. If the file already exists, the table of values is appended to the end of the file to allow multiple tables of energy and force to be included in one file.

The energy and force values are computed at distances from inner to outer for 2 interacting atoms forming a bond of type btype, using the appropriate *bond_coeff* coefficients. N evenly spaced distances are used.

For example, for N = 7, inner = 1.0, and outer = 4.0, values are computed at r = 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0.

The file is written in the format used as input for the *bond_style table* option with *keyword* as the section name. Each line written to the file lists an index number (1-N), a distance (in distance units), an energy (in energy units), and a force (in force units).

15.8.4 Restrictions

All force field coefficients for bond and other kinds of interactions must be set before this command can be invoked.

Due to how the bond force is computed, an inner value > 0.0 must be specified even if the potential has a finite value at r = 0.0.

15.8.5 Related commands

bond_style table, *bond_style*, *bond_coeff*

Default: none

15.9 boundary command

15.9.1 Syntax

```
boundary x y z
```

- x,y,z = *p* or *s* or *f* or *m*, one or two letters

```
p is periodic
f is non-periodic and fixed
s is non-periodic and shrink-wrapped
m is non-periodic and shrink-wrapped with a minimum value
```

15.9.2 Examples

```
boundary p p f
boundary p fs p
boundary s f fm
```

15.9.3 Description

Set the style of boundaries for the global simulation box in each dimension. A single letter assigns the same style to both the lower and upper face of the box. Two letters assigns the first style to the lower face and the second style to the upper face. The initial size of the simulation box is set by the *read_data*, *read_restart*, or *create_box* commands.

The style *p* means the box is periodic, so that particles interact across the boundary, and they can exit one end of the box and re-enter the other end. A periodic dimension can change in size due to constant pressure boundary conditions or box deformation (see the *fix npt* and *fix deform* commands). The *p* style must be applied to both faces of a dimension.

The styles *f*, *s*, and *m* mean the box is non-periodic, so that particles do not interact across the boundary and do not move from one side of the box to the other.

For style *f*, the position of the face is fixed. If an atom moves outside the face it will be deleted on the next timestep that reneighboring occurs. This will typically generate an error unless you have set the *thermo_modify lost* option to allow for lost atoms.

For style *s*, the position of the face is set so as to encompass the atoms in that dimension (shrink-wrapping), no matter how far they move. Note that when the difference between the current box dimensions and the shrink-wrap box dimensions is large, this can lead to lost atoms at the beginning of a run when running in parallel. This is due to the large change in the (global) box dimensions also causing significant changes in the individual sub-domain sizes. If these changes are farther than the communication cutoff, atoms will be lost. This is best addressed by setting initial box dimensions to match the shrink-wrapped dimensions more closely, by using *m* style boundaries (see below).

For style *m*, shrink-wrapping occurs, but is bounded by the value specified in the data or restart file or set by the *create_box* command. For example, if the upper z face has a value of 50.0 in the data file, the face will always be positioned at 50.0 or above, even if the maximum z-extent of all the atoms becomes less than 50.0. This can be useful if you start a simulation with an empty box or if you wish to leave room on one side of the box, e.g. for atoms to evaporate from a surface.

For triclinic (non-orthogonal) simulation boxes, if the 2nd dimension of a tilt factor (e.g. y for xy) is periodic, then the periodicity is enforced with the tilt factor offset. If the 1st dimension is shrink-wrapped, then the shrink wrapping is applied to the tilted box face, to encompass the atoms. E.g. for a positive xy tilt, the xlo and xhi faces of the box are planes tilting in the +y direction as y increases. These tilted planes are shrink-wrapped around the atoms to determine the x extent of the box.

See the *Howto triclinic* doc page for a geometric description of triclinic boxes, as defined by LAMMPS, and how to transform these parameters to and from other commonly used triclinic representations.

15.9.4 Restrictions

This command cannot be used after the simulation box is defined by a *read_data* or *create_box* command or *read_restart* command. See the *change_box* command for how to change the simulation box boundaries after it has been defined.

For 2d simulations, the z dimension must be periodic.

15.9.5 Related commands

See the *thermo_modify* command for a discussion of lost atoms.

15.9.6 Default

```
boundary p p p
```

15.10 box command

15.10.1 Syntax

```
box keyword value ...
```

- one or more keyword/value pairs may be appended
- keyword = *tilt*

```
tilt value = small or large
```

15.10.2 Examples

```
box tilt large
box tilt small
```

15.10.3 Description

Set attributes of the simulation box.

For triclinic (non-orthogonal) simulation boxes, the *tilt* keyword allows simulation domains to be created with arbitrary tilt factors, e.g. via the *create_box* or *read_data* commands. Tilt factors determine how skewed the triclinic box is; see the *Howto triclinic* doc page for a discussion of triclinic boxes in LAMMPS.

LAMMPS normally requires that no tilt factor can skew the box more than half the distance of the parallel box length, which is the 1st dimension in the tilt factor (x for xz). If *tilt* is set to *small*, which is the default, then an error will be generated if a box is created which exceeds this limit. If *tilt* is set to *large*, then no limit is enforced. You can create a box with any tilt factors you wish.

Note that if a simulation box has a large tilt factor, LAMMPS will run less efficiently, due to the large volume of communication needed to acquire ghost atoms around a processor's irregular-shaped sub-domain. For extreme values of tilt, LAMMPS may also lose atoms and generate an error.

15.10.4 Restrictions

This command cannot be used after the simulation box is defined by a *read_data* or *create_box* command or *read_restart* command.

Related commands: none

15.10.5 Default

The default value is tilt = small.

15.11 change_box command

15.11.1 Syntax

```
change_box group-ID parameter args ... keyword args ...
```

- group-ID = ID of group of atoms to (optionally) displace
- one or more parameter/arg pairs may be appended

```
parameter = x or y or z or xy or xz or yz or boundary or ortho or␣
↪triclinic or set or remap
  x, y, z args = style value(s)
    style = final or delta or scale or volume
      final values = lo hi
        lo hi = box boundaries after displacement (distance units)
```

```
      delta values = dlo dhi
        dlo dhi = change in box boundaries after displacement (distance␣
↪units)
      scale values = factor
        factor = multiplicative factor for change in box length after␣
↪displacement
      volume value = none = adjust this dim to preserve volume of system
  xy, xz, yz args = style value
    style = final or delta
      final value = tilt
        tilt = tilt factor after displacement (distance units)
      delta value = dtilt
        dtilt = change in tilt factor after displacement (distance units)
  boundary args = x y z
    x,y,z = p or s or f or m, one or two letters
    p is periodic
    f is non-periodic and fixed
    s is non-periodic and shrink-wrapped
    m is non-periodic and shrink-wrapped with a minimum value
  ortho args = none = change box to orthogonal
  triclinic args = none = change box to triclinic
  set args = none = store state of current box
  remap args = none = remap atom coords from last saved state to current␣
↪box
```

- zero or more keyword/value pairs may be appended
- keyword = *units*

```
  units value = lattice or box
    lattice = distances are defined in lattice units
    box = distances are defined in simulation box units
```

15.11.2 Examples

```
change_box all xy final -2.0 z final 0.0 5.0 boundary p p f remap units box
change_box all x scale 1.1 y volume z volume remap
```

15.11.3 Description

Change the volume and/or shape and/or boundary conditions for the simulation box. Orthogonal simulation boxes have 3 adjustable size parameters (x,y,z). Triclinic (non-orthogonal) simulation boxes have 6 adjustable size/shape parameters (x,y,z,xy,xz,yz). Any or all of them can be adjusted independently by this command. Thus it can be used to expand or contract a box, or to apply a shear strain to a non-orthogonal box. It can also be used to change the boundary conditions for the simulation box, similar to the *boundary* command.

The size and shape of the initial simulation box are specified by the *create_box* or *read_data* or *read_restart* command used to setup the simulation. The size and shape may be altered by subsequent runs, e.g. by use of the *fix npt* or *fix deform* commands. The *create_box*, *read data*, and *read_restart* commands also determine whether the simulation box is orthogonal or triclinic and their doc pages explain the meaning of the xy,xz,yz tilt factors.

See the *Howto triclinic* doc page for a geometric description of triclinic boxes, as defined by LAMMPS, and how to transform these parameters to and from other commonly used triclinic representations.

The keywords used in this command are applied sequentially to the simulation box and the atoms in it, in the order specified.

Before the sequence of keywords are invoked, the current box size/shape is stored, in case a *remap* keyword is used to map the atom coordinates from a previously stored box size/shape to the current one.

After all the keywords have been processed, any shrink-wrap boundary conditions are invoked (see the *boundary* command) which may change simulation box boundaries, and atoms are migrated to new owning processors.

Note: This means that you cannot use the change_box command to enlarge a shrink-wrapped box, e.g. to make room to insert more atoms via the *create_atoms* command, because the simulation box will be re-shrink-wrapped before the change_box command completes. Instead you could do something like this, assuming the simulation box is non-periodic and atoms extend from 0 to 20 in all dimensions:

```
change_box all x final -10 20
create_atoms 1 single -5 5 5       # this will fail to insert an atom

change_box all x final -10 20 boundary f s s
create_atoms 1 single -5 5 5
change_box all boundary s s s      # this will work
```

Note: Unlike the earlier "displace_box" version of this command, atom remapping is NOT performed by default. This command allows remapping to be done in a more general way, exactly when you specify it (zero or more times) in the sequence of transformations. Thus if you do not use the *remap* keyword, atom coordinates will not be changed even if the box size/shape changes. If a uniformly strained state is desired, the *remap* keyword should be specified.

Note: It is possible to lose atoms with this command. E.g. by changing the box without remapping the atoms, and having atoms end up outside of non-periodic boundaries. It is also possible to alter bonds between atoms straddling a boundary in bad ways. E.g. by converting a boundary from periodic to non-periodic. It is also possible when remapping atoms to put them (nearly) on top of each other. E.g. by converting a boundary from non-periodic to periodic. All of these will typically lead to bad dynamics and/or generate error messages.

Note: The simulation box size/shape can be changed by arbitrarily large amounts by this command. This is not a problem, except that the mapping of processors to the simulation box is not changed from its initial 3d configuration; see the *processors* command. Thus, if the box size/shape changes dramatically, the mapping of processors to the simulation box may not end up as optimal as the initial mapping attempted to be.

Note: Because the keywords used in this command are applied one at a time to the simulation box and the atoms in it, care must be taken with triclinic cells to avoid exceeding the limits on skew after each transformation in the sequence. If skew is exceeded before the final transformation this can be avoided by changing the order of the sequence, or breaking the transformation into two or more smaller transformations. For more information on the allowed limits for box skew see the discussion on triclinic boxes on *Howto triclinic* doc page.

For the *x*, *y*, and *z* parameters, this is the meaning of their styles and values.

For style *final*, the final lo and hi box boundaries of a dimension are specified. The values can be in lattice or box distance units. See the discussion of the units keyword below.

For style *delta*, plus or minus changes in the lo/hi box boundaries of a dimension are specified. The values can be in lattice or box distance units. See the discussion of the units keyword below.

For style *scale*, a multiplicative factor to apply to the box length of a dimension is specified. For example, if the initial box length is 10, and the factor is 1.1, then the final box length will be 11. A factor less than 1.0 means compression.

The *volume* style changes the specified dimension in such a way that the overall box volume remains constant with respect to the operation performed by the preceding keyword. The *volume* style can only be used following a keyword that changed the volume, which is any of the *x*, *y*, *z* keywords. If the preceding keyword "key" had a *volume* style, then both it and the current keyword apply to the keyword preceding "key". I.e. this sequence of keywords is allowed:

```
change_box all x scale 1.1 y volume z volume
```

The *volume* style changes the associated dimension so that the overall box volume is unchanged relative to its value before the preceding keyword was invoked.

If the following command is used, then the z box length will shrink by the same 1.1 factor the x box length was increased by:

```
change_box all x scale 1.1 z volume
```

If the following command is used, then the y,z box lengths will each shrink by sqrt(1.1) to keep the volume constant. In this case, the y,z box lengths shrink so as to keep their relative aspect ratio constant:

```
change_box all x scale 1.1 y volume z volume
```

If the following command is used, then the final box will be a factor of 10% larger in x and y, and a factor of 21% smaller in z, so as to keep the volume constant:

```
change_box all x scale 1.1 z volume y scale 1.1 z volume
```

Note: For solids or liquids, when one dimension of the box is expanded, it may be physically undesirable to hold the other 2 box lengths constant since that implies a density change. For solids, adjusting the other dimensions via the *volume* style may make physical sense (just as for a liquid), but may not be correct for materials and potentials whose Poisson ratio is not 0.5.

For the *scale* and *volume* styles, the box length is expanded or compressed around its mid point.

For the *xy*, *xz*, and *yz* parameters, this is the meaning of their styles and values. Note that changing the tilt factors of a triclinic box does not change its volume.

For style *final*, the final tilt factor is specified. The value can be in lattice or box distance units. See the discussion of the units keyword below.

For style *delta*, a plus or minus change in the tilt factor is specified. The value can be in lattice or box distance units. See the discussion of the units keyword below.

All of these styles change the xy, xz, yz tilt factors. In LAMMPS, tilt factors (xy,xz,yz) for triclinic boxes are required to be no more than half the distance of the parallel box length. For example, if xlo = 2 and xhi = 12, then the x box length is 10 and the xy tilt factor must be between -5 and 5. Similarly, both xz and yz must be between -(xhi-xlo)/2 and +(yhi-ylo)/2. Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = . . . , -15, -5, 5, 15, 25, . . . are all equivalent. Any tilt factor specified by this command must be within these limits.

The *boundary* keyword takes arguments that have exactly the same meaning as they do for the *boundary* command. In each dimension, a single letter assigns the same style to both the lower and upper face of the box. Two letters assigns the first style to the lower face and the second style to the upper face.

The style *p* means the box is periodic; the other styles mean non-periodic. For style *f*, the position of the face is fixed. For style *s*, the position of the face is set so as to encompass the atoms in that dimension (shrink-wrapping), no matter how far they move. For style *m*, shrink-wrapping occurs, but is bounded by the current box edge in that dimension, so that the box will become no smaller. See the *boundary* command for more explanation of these style options.

Note that the "boundary" command itself can only be used before the simulation box is defined via a *read_data* or *create_box* or *read_restart* command. This command allows the boundary conditions to be changed later in your input script. Also note that the *read_restart* will change boundary conditions to match what is stored in the restart file. So if you wish to change them, you should use the change_box command after the read_restart command.

The *ortho* and *triclinic* keywords convert the simulation box to be orthogonal or triclinic (non-orthogonal).

The simulation box is defined as either orthogonal or triclinic when it is created via the *create_box*, *read_data*, or *read_restart* commands.

These keywords allow you to toggle the existing simulation box from orthogonal to triclinic and vice versa. For example, an initial equilibration simulation can be run in an orthogonal box, the box can be toggled to triclinic, and then a *non-equilibrium MD (NEMD) simulation* can be run with deformation via the *fix deform* command.

If the simulation box is currently triclinic and has non-zero tilt in xy, yz, or xz, then it cannot be converted to an orthogonal box.

The *set* keyword saves the current box size/shape. This can be useful if you wish to use the *remap* keyword more than once or if you wish it to be applied to an intermediate box size/shape in a sequence of keyword operations. Note that the box size/shape is saved before any of the keywords are processed, i.e. the box size/shape at the time the create_box command is encountered in the input script.

The *remap* keyword remaps atom coordinates from the last saved box size/shape to the current box state. For example, if you stretch the box in the x dimension or tilt it in the xy plane via the *x* and *xy* keywords, then the *remap* command will dilate or tilt the atoms to conform to the new box size/shape, as if the atoms moved with the box as it deformed.

Note that this operation is performed without regard to periodic boundaries. Also, any shrink-wrapping of non-periodic boundaries (see the *boundary* command) occurs after all keywords, including this one, have been processed.

Only atoms in the specified group are remapped.

The *units* keyword determines the meaning of the distance units used to define various arguments. A *box* value selects standard distance units as defined by the *units* command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacing.

15.11.4 Restrictions

If you use the *ortho* or *triclinic* keywords, then at the point in the input script when this command is issued, no *dumps* can be active, nor can a *fix deform* be active. This is because these commands test whether the simulation box is orthogonal when they are first issued. Note that these commands can be used in your script before a change_box command is issued, so long as an *undump* or *unfix* command is also used to turn them off.

15.11.5 Related commands

fix deform, *boundary*

15.11.6 Default

The option default is units = lattice.

15.12 clear command

15.12.1 Syntax

```
clear
```

15.12.2 Examples

```
(commands for 1st simulation)
clear
(commands for 2nd simulation)
```

15.12.3 Description

This command deletes all atoms, restores all settings to their default values, and frees all memory allocated by LAMMPS. Once a clear command has been executed, it is almost as if LAMMPS were starting over, with only the exceptions noted below. This command enables multiple jobs to be run sequentially from one input script.

These settings are not affected by a clear command: the working directory (*shell* command), log file status (*log* command), echo status (*echo* command), and input script variables (*variable* command).

15.12.4 Restrictions

none

Related commands: none

Default: none

15.13 comm_modify command

15.13.1 Syntax

```
comm_modify keyword value ...
```

- zero or more keyword/value pairs may be appended
- keyword = *mode* or *cutoff* or *cutoff/multi* or *group* or *vel*

```
mode value = single or multi = communicate atoms within a single or␣
↪multiple distances
cutoff value = Rcut (distance units) = communicate atoms from this far␣
↪away
cutoff/multi type value
   type = atom type or type range (supports asterisk notation)
   value = Rcut (distance units) = communicate atoms for selected types␣
↪from this far away
group value = group-ID = only communicate atoms in the group
vel value = yes or no = do or do not communicate velocity info with ghost␣
↪atoms
```

15.13.2 Examples

```
comm_modify mode multi
comm_modify mode multi group solvent
comm_modift mode multi cutoff/multi 1 10.0 cutoff/multi 2*4 15.0
comm_modify vel yes
comm_modify mode single cutoff 5.0 vel yes
comm_modify cutoff/multi * 0.0
```

15.13.3 Description

This command sets parameters that affect the inter-processor communication of atom information that occurs each timestep as coordinates and other properties are exchanged between neighboring processors and stored as properties of ghost atoms.

Note: These options apply to the currently defined comm style. When you specify a *comm_style* or *read_restart* command, all communication settings are restored to their default or stored values, including those previously reset by a comm_modify command. Thus if your input script specifies a comm_style or read_restart command, you should use the comm_modify command after it.

The *mode* keyword determines whether a single or multiple cutoff distances are used to determine which atoms to communicate.

The default mode is *single* which means each processor acquires information for ghost atoms that are within a single distance from its sub-domain. The distance is by default the maximum of the neighbor cutoff across all atom type pairs.

For many systems this is an efficient algorithm, but for systems with widely varying cutoffs for different type pairs, the *multi* mode can be faster. In this case, each atom type is assigned its own distance cutoff for communication purposes,

and fewer atoms will be communicated. See the *neighbor multi* command for a neighbor list construction option that may also be beneficial for simulations of this kind.

The *cutoff* keyword allows you to extend the ghost cutoff distance for communication mode *single*, which is the distance from the borders of a processor's sub-domain at which ghost atoms are acquired from other processors. By default the ghost cutoff = neighbor cutoff = pairwise force cutoff + neighbor skin. See the *neighbor* command for more information about the skin distance. If the specified Rcut is greater than the neighbor cutoff, then extra ghost atoms will be acquired. If the provided cutoff is smaller, the provided value will be ignored, the ghost cutoff is set to the neighbor cutoff and a warning will be printed. Specifying a cutoff value of 0.0 will reset any previous value to the default. If bonded interactions exist and equilibrium bond length information is available, then also a heuristic based on that bond length is computed. It is used as communication cutoff, if there is no pair style present and no *comm_modify cutoff* command used. Otherwise a warning is printed, if this bond based estimate is larger than the communication cutoff used. A

The *cutoff/multi* option is equivalent to *cutoff*, but applies to communication mode *multi* instead. Since in this case the communication cutoffs are determined per atom type, a type specifier is needed and cutoff for one or multiple types can be extended. Also ranges of types using the usual asterisk notation can be given.

These are simulation scenarios in which it may be useful or even necessary to set a ghost cutoff > neighbor cutoff:

- a single polymer chain with bond interactions, but no pairwise interactions
- bonded interactions (e.g. dihedrals) extend further than the pairwise cutoff
- ghost atoms beyond the pairwise cutoff are needed for some computation

In the first scenario, a pairwise potential is not defined. Thus the pairwise neighbor cutoff will be 0.0. But ghost atoms are still needed for computing bond, angle, etc interactions between atoms on different processors, or when the interaction straddles a periodic boundary.

The appropriate ghost cutoff depends on the *newton bond* setting. For newton bond *off*, the distance needs to be the furthest distance between any two atoms in the bond, angle, etc. E.g. the distance between 1-4 atoms in a dihedral. For newton bond *on*, the distance between the central atom in the bond, angle, etc and any other atom is sufficient. E.g. the distance between 2-4 atoms in a dihedral.

In the second scenario, a pairwise potential is defined, but its neighbor cutoff is not sufficiently long enough to enable bond, angle, etc terms to be computed. As in the previous scenario, an appropriate ghost cutoff should be set.

In the last scenario, a *fix* or *compute* or *pairwise potential* needs to calculate with ghost atoms beyond the normal pairwise cutoff for some computation it performs (e.g. locate neighbors of ghost atoms in a multibody pair potential). Setting the ghost cutoff appropriately can insure it will find the needed atoms.

Note: In these scenarios, if you do not set the ghost cutoff long enough, and if there is only one processor in a periodic dimension (e.g. you are running in serial), then LAMMPS may "find" the atom it is looking for (e.g. the partner atom in a bond), that is on the far side of the simulation box, across a periodic boundary. This will typically lead to bad dynamics (i.e. the bond length is now the simulation box length). To detect if this is happening, see the *neigh_modify cluster* command.

The *group* keyword will limit communication to atoms in the specified group. This can be useful for models where no ghost atoms are needed for some kinds of particles. All atoms (not just those in the specified group) will still migrate to new processors as they move. The group specified with this option must also be specified via the *atom_modify first* command.

The *vel* keyword enables velocity information to be communicated with ghost particles. Depending on the *atom_style*, velocity info includes the translational velocity, angular velocity, and angular momentum of a particle. If the *vel* option is set to *yes*, then ghost atoms store these quantities; if *no* then they do not. The *yes* setting is needed by some pair styles which require the velocity state of both the I and J particles to compute a pairwise I,J interaction, as well as by some compute and fix commands.

Note that if the *fix deform* command is being used with its "remap v" option enabled, then the velocities for ghost atoms (in the fix deform group) mirrored across a periodic boundary will also include components due to any velocity shift that occurs across that boundary (e.g. due to dilation or shear).

15.13.4 Restrictions

Communication mode *multi* is currently only available for *comm_style brick*.

15.13.5 Related commands

comm_style, *neighbor*

15.13.6 Default

The option defaults are mode = single, group = all, cutoff = 0.0, vel = no. The cutoff default of 0.0 means that ghost cutoff = neighbor cutoff = pairwise force cutoff + neighbor skin.

15.14 comm_style command

15.14.1 Syntax

```
comm_style style
```

- style = *brick* or *tiled*

15.14.2 Examples

```
comm_style brick
comm_style tiled
```

15.14.3 Description

This command sets the style of inter-processor communication of atom information that occurs each timestep as coordinates and other properties are exchanged between neighboring processors and stored as properties of ghost atoms.

For the default *brick* style, the domain decomposition used by LAMMPS to partition the simulation box must be a regular 3d grid of bricks, one per processor. Each processor communicates with its 6 Cartesian neighbors in the grid to acquire information for nearby atoms.

For the *tiled* style, a more general domain decomposition can be used, as triggered by the *balance* or *fix balance* commands. The simulation box can be partitioned into non-overlapping rectangular-shaped "tiles" or varying sizes and shapes. Again there is one tile per processor. To acquire information for nearby atoms, communication must now be done with a more complex pattern of neighboring processors.

Note that this command does not actually define a partitioning of the simulation box (a domain decomposition), rather it determines what kinds of decompositions are allowed and the pattern of communication used to enable the decomposition. A decomposition is created when the simulation box is first created, via the *create_box* or *read_data* or

read_restart commands. For both the *brick* and *tiled* styles, the initial decomposition will be the same, as described by *create_box* and *processors* commands. The decomposition can be changed via the *balance* or *fix balance* commands.

15.14.4 Restrictions

Communication style *tiled* cannot be used with *triclinic* simulation cells.

15.14.5 Related commands

comm_modify, *processors*, *balance*, *fix balance*

15.14.6 Default

The default style is brick.

15.15 compute command

15.15.1 Syntax

```
compute ID group-ID style args
```

- ID = user-assigned name for the computation
- group-ID = ID of the group of atoms to perform the computation on
- style = one of a list of possible style names (see below)
- args = arguments used by a particular style

15.15.2 Examples

```
compute 1 all temp
compute newtemp flow temp/partial 1 1 0
compute 3 all ke/atom
```

15.15.3 Description

Define a computation that will be performed on a group of atoms. Quantities calculated by a compute are instantaneous values, meaning they are calculated from information about atoms on the current timestep or iteration, though a compute may internally store some information about a previous state of the system. Defining a compute does not perform a computation. Instead computes are invoked by other LAMMPS commands as needed, e.g. to calculate a temperature needed for a thermostat fix or to generate thermodynamic or dump file output. See the *Howto output* doc page for a summary of various LAMMPS output options, many of which involve computes.

The ID of a compute can only contain alphanumeric characters and underscores.

Computes calculate one of three styles of quantities: global, per-atom, or local. A global quantity is one or more system-wide values, e.g. the temperature of the system. A per-atom quantity is one or more values per atom, e.g.

the kinetic energy of each atom. Per-atom values are set to 0.0 for atoms not in the specified compute group. Local quantities are calculated by each processor based on the atoms it owns, but there may be zero or more per atom, e.g. a list of bond distances. Computes that produce per-atom quantities have the word "atom" in their style, e.g. *ke/atom*. Computes that produce local quantities have the word "local" in their style, e.g. *bond/local*. Styles with neither "atom" or "local" in their style produce global quantities.

Note that a single compute can produce either global or per-atom or local quantities, but not both global and per-atom. It can produce local quantities in tandem with global or per-atom quantities. The compute doc page will explain.

Global, per-atom, and local quantities each come in three kinds: a single scalar value, a vector of values, or a 2d array of values. The doc page for each compute describes the style and kind of values it produces, e.g. a per-atom vector. Some computes produce more than one kind of a single style, e.g. a global scalar and a global vector.

When a compute quantity is accessed, as in many of the output commands discussed below, it can be referenced via the following bracket notation, where ID is the ID of the compute:

c_ID	entire scalar, vector, or array
c_ID[I]	one element of vector, one column of array
c_ID[I][J]	one element of array

In other words, using one bracket reduces the dimension of the quantity once (vector -> scalar, array -> vector). Using two brackets reduces the dimension twice (array -> scalar). Thus a command that uses scalar compute values as input can also process elements of a vector or array.

Note that commands and *variables* which use compute quantities typically do not allow for all kinds, e.g. a command may require a vector of values, not a scalar. This means there is no ambiguity about referring to a compute quantity as c_ID even if it produces, for example, both a scalar and vector. The doc pages for various commands explain the details.

In LAMMPS, the values generated by a compute can be used in several ways:

- The results of computes that calculate a global temperature or pressure can be used by fixes that do thermostatting or barostatting or when atom velocities are created.
- Global values can be output via the *thermo_style custom* or *fix ave/time* command. Or the values can be referenced in a *variable equal* or *variable atom* command.
- Per-atom values can be output via the *dump custom* command. Or they can be time-averaged via the *fix ave/atom* command or reduced by the *compute reduce* command. Or the per-atom values can be referenced in an *atom-style variable*.
- Local values can be reduced by the *compute reduce* command, or histogrammed by the *fix ave/histo* command, or output by the *dump local* command.

The results of computes that calculate global quantities can be either "intensive" or "extensive" values. Intensive means the value is independent of the number of atoms in the simulation, e.g. temperature. Extensive means the value scales with the number of atoms in the simulation, e.g. total rotational kinetic energy. *Thermodynamic output* will normalize extensive values by the number of atoms in the system, depending on the "thermo_modify norm" setting. It will not normalize intensive values. If a compute value is accessed in another way, e.g. by a *variable*, you may want to know whether it is an intensive or extensive value. See the doc page for individual computes for further info.

LAMMPS creates its own computes internally for thermodynamic output. Three computes are always created, named "thermo_temp", "thermo_press", and "thermo_pe", as if these commands had been invoked in the input script:

```
compute thermo_temp all temp
compute thermo_press all pressure thermo_temp
compute thermo_pe all pe
```

Additional computes for other quantities are created if the thermo style requires it. See the documentation for the *thermo_style* command.

Fixes that calculate temperature or pressure, i.e. for thermostatting or barostatting, may also create computes. These are discussed in the documentation for specific *fix* commands.

In all these cases, the default computes LAMMPS creates can be replaced by computes defined by the user in the input script, as described by the *thermo_modify* and *fix modify* commands.

Properties of either a default or user-defined compute can be modified via the *compute_modify* command.

Computes can be deleted with the *uncompute* command.

Code for new computes can be added to LAMMPS; see the *Modify* doc page for details. The results of their calculations accessed in the various ways described above.

Each compute style has its own doc page which describes its arguments and what it does. Here is an alphabetic list of compute styles available in LAMMPS. They are also listed in more compact form on the *Commands compute* doc page.

There are also additional accelerated compute styles included in the LAMMPS distribution for faster performance on CPUs, GPUs, and KNLs. The individual style names on the *Commands compute* doc page are followed by one or more of (g,i,k,o,t) to indicate which accelerated styles exist.

- *ackland/atom* - determines the local lattice structure based on the Ackland formulation
- *adf* - angular distribution function of triples of atoms
- *aggregate/atom* - aggregate ID for each atom
- *angle* - energy of each angle sub-style
- *angle/local* - theta and energy of each angle
- *angmom/chunk* - angular momentum for each chunk
- *basal/atom* - calculates the hexagonal close-packed "c" lattice vector of each atom
- *body/local* - attributes of body sub-particles
- *bond* - energy of each bond sub-style
- *bond/local* - distance and energy of each bond
- *centro/atom* - centro-symmetry parameter for each atom
- *centroid/stress/atom* - centroid based stress tensor for each atom
- *chunk/atom* - assign chunk IDs to each atom
- *chunk/spread/atom* - spreads chunk values to each atom in chunk
- *cluster/atom* - cluster ID for each atom
- *cna/atom* - common neighbor analysis (CNA) for each atom
- *cnp/atom* - common neighborhood parameter (CNP) for each atom
- *com* - center-of-mass of group of atoms
- *com/chunk* - center-of-mass for each chunk

- *contact/atom* - contact count for each spherical particle
- *coord/atom* - coordination number for each atom
- *damage/atom* - Peridynamic damage for each atom
- *dihedral* - energy of each dihedral sub-style
- *dihedral/local* - angle of each dihedral
- *dilatation/atom* - Peridynamic dilatation for each atom
- *dipole/chunk* - dipole vector and total dipole for each chunk
- *displace/atom* - displacement of each atom
- *dpd* -
- *dpd/atom* -
- *edpd/temp/atom* - per-atom temperature for each eDPD particle in a group
- *entropy/atom* - pair entropy fingerprint of each atom
- *erotate/asphere* - rotational energy of aspherical particles
- *erotate/rigid* - rotational energy of rigid bodies
- *erotate/sphere* - rotational energy of spherical particles
- *erotate/sphere/atom* - rotational energy for each spherical particle
- *event/displace* - detect event on atom displacement
- *fep* -
- *force/tally* -
- *fragment/atom* - fragment ID for each atom
- *global/atom* -
- *group/group* - energy/force between two groups of atoms
- *gyration* - radius of gyration of group of atoms
- *gyration/chunk* - radius of gyration for each chunk
- *gyration/shape* - shape parameters from gyration tensor
- *gyration/shape/chunk* - shape parameters from gyration tensor for each chunk
- *heat/flux* - heat flux through a group of atoms
- *heat/flux/tally* -
- *hexorder/atom* - bond orientational order parameter q6
- *hma* - harmonically mapped averaging for atomic crystals
- *improper* - energy of each improper sub-style
- *improper/local* - angle of each improper
- *inertia/chunk* - inertia tensor for each chunk
- *ke* - translational kinetic energy
- *ke/atom* - kinetic energy for each atom
- *ke/atom/eff* - per-atom translational and radial kinetic energy in the electron force field model

- *ke/eff* - kinetic energy of a group of nuclei and electrons in the electron force field model
- *ke/rigid* - translational kinetic energy of rigid bodies
- *meso/e/atom* - per-atom internal energy of Smooth-Particle Hydrodynamics atoms
- *meso/rho/atom* - per-atom mesoscopic density of Smooth-Particle Hydrodynamics atoms
- *meso/t/atom* - per-atom internal temperature of Smooth-Particle Hydrodynamics atoms
- *momentum* - translational momentum
- *msd* - mean-squared displacement of group of atoms
- *msd/chunk* - mean-squared displacement for each chunk
- *msd/nongauss* - MSD and non-Gaussian parameter of group of atoms
- *omega/chunk* - angular velocity for each chunk
- *orientorder/atom* - Steinhardt bond orientational order parameters Ql
- *pair* - values computed by a pair style
- *pair/local* - distance/energy/force of each pairwise interaction
- *pe* - potential energy
- *pe/atom* - potential energy for each atom
- *pe/mol/tally* -
- *pe/tally* -
- *plasticity/atom* - Peridynamic plasticity for each atom
- *pressure* - total pressure and pressure tensor
- *pressure/cylinder* - pressure tensor in cylindrical coordinates
- *pressure/uef* - pressure tensor in the reference frame of an applied flow field
- *property/atom* - convert atom attributes to per-atom vectors/arrays
- *property/chunk* - extract various per-chunk attributes
- *property/local* - convert local attributes to localvectors/arrays
- *ptm/atom* - determines the local lattice structure based on the Polyhedral Template Matching method
- *rdf* - radial distribution function g(r) histogram of group of atoms
- *reduce* - combine per-atom quantities into a single global value
- *reduce/chunk* - reduce per-atom quantities within each chunk
- *reduce/region* - same as compute reduce, within a region
- *rigid/local* - extract rigid body attributes
- *saed* - electron diffraction intensity on a mesh of reciprocal lattice nodes
- *slice* - extract values from global vector or array
- *smd/contact/radius* -
- *smd/damage* - damage status of SPH particles in Smooth Mach Dynamics
- *smd/hourglass/error* -
- *smd/internal/energy* - per-particle enthalpy in Smooth Mach Dynamics

- *smd/plastic/strain* - equivalent plastic strain per particle in Smooth Mach Dynamics
- *smd/plastic/strain/rate* - time rate of the equivalent plastic strain in Smooth Mach Dynamics
- *smd/rho* - per-particle mass density in Smooth Mach Dynamics
- *smd/tlsph/defgrad* - deformation gradient in Smooth Mach Dynamics
- *smd/tlsph/dt* - CFL-stable time increment per particle in Smooth Mach Dynamics
- *smd/tlsph/num/neighs* -
- *smd/tlsph/shape* -
- *smd/tlsph/strain* -
- *smd/tlsph/strain/rate* -
- *smd/tlsph/stress* - per-particle Cauchy stress tensor for SPH particles
- *smd/triangle/vertices* -
- *smd/ulsph/num/neighs* -
- *smd/ulsph/strain* -
- *smd/ulsph/strain/rate* -
- *smd/ulsph/stress* - per-particle Cauchy stress tensor and von Mises equivalent stress in Smooth Mach Dynamics
- *smd/vol* - per-particle volumes and their sum in Smooth Mach Dynamics
- *snap* - bispectrum components and related quantities for a group of atoms
- *sna/atom* - bispectrum components for each atom
- *snad/atom* - derivative of bispectrum components for each atom
- *snav/atom* - virial contribution from bispectrum components for each atom
- *spin* - magnetic quantities for a system of atoms having spins
- *stress/atom* - stress tensor for each atom
- *stress/mop* - normal components of the local stress tensor using the method of planes
- *stress/mop/profile* - profile of the normal components of the local stress tensor using the method of planes
- *stress/tally* -
- *tdpd/cc/atom* - per-atom chemical concentration of a specified species for each tDPD particle
- *temp* - temperature of group of atoms
- *temp/asphere* - temperature of aspherical particles
- *temp/body* - temperature of body particles
- *temp/chunk* - temperature of each chunk
- *temp/com* - temperature after subtracting center-of-mass velocity
- *temp/cs* - temperature based on the center-of-mass velocity of atom pairs that are bonded to each other
- *temp/deform* - temperature excluding box deformation velocity
- *temp/deform/eff* - temperature excluding box deformation velocity in the electron force field model
- *temp/drude* - temperature of Core-Drude pairs
- *temp/eff* - temperature of a group of nuclei and electrons in the electron force field model

- *temp/partial* - temperature excluding one or more dimensions of velocity
- *temp/profile* - temperature excluding a binned velocity profile
- *temp/ramp* - temperature excluding ramped velocity component
- *temp/region* - temperature of a region of atoms
- *temp/region/eff* - temperature of a region of nuclei and electrons in the electron force field model
- *temp/rotate* - temperature of a group of atoms after subtracting out their center-of-mass and angular velocities
- *temp/sphere* - temperature of spherical particles
- *temp/uef* - kinetic energy tensor in the reference frame of an applied flow field
- *ti* - thermodynamic integration free energy values
- *torque/chunk* - torque applied on each chunk
- *vacf* - velocity auto-correlation function of group of atoms
- *vcm/chunk* - velocity of center-of-mass for each chunk
- *voronoi/atom* - Voronoi volume and neighbors for each atom
- *xrd* - x-ray diffraction intensity on a mesh of reciprocal lattice nodes

15.15.4 Restrictions

none

15.15.5 Related commands

uncompute, *compute_modify*, *fix ave/atom*, *fix ave/time*, *fix ave/histo*

Default: none

15.16 compute_modify command

15.16.1 Syntax

```
compute_modify compute-ID keyword value ...
```

- compute-ID = ID of the compute to modify
- one or more keyword/value pairs may be listed
- keyword = *extra/dof* or *extra* or *dynamic/dof* or *dynamic*

```
extra/dof value = N
  N = # of extra degrees of freedom to subtract
extra syntax is identical to extra/dof, will be disabled at some point
dynamic/dof value = yes or no
  yes/no = do or do not re-compute the number of degrees of freedom (DOF)␣
↪contributing to the temperature
dynamic syntax is identical to dynamic/dof, will be disabled at some point
```

15.16.2 Examples

```
compute_modify myTemp extra/dof 0
compute_modify newtemp dynamic/dof yes extra/dof 600
```

15.16.3 Description

Modify one or more parameters of a previously defined compute. Not all compute styles support all parameters.

The *extra/dof* or *extra* keyword refers to how many degrees-of-freedom are subtracted (typically from 3N) as a normalizing factor in a temperature computation. Only computes that compute a temperature use this option. The default is 2 or 3 for *2d or 3d systems* which is a correction factor for an ensemble of velocities with zero total linear momentum. For compute temp/partial, if one or more velocity components are excluded, the value used for *extra* is scaled accordingly. You can use a negative number for the *extra* parameter if you need to add degrees-of-freedom. See the *compute temp/asphere* command for an example.

The *dynamic/dof* or *dynamic* keyword determines whether the number of atoms N in the compute group and their associated degrees of freedom are re-computed each time a temperature is computed. Only compute styles that calculate a temperature use this option. By default, N and their DOF are assumed to be constant. If you are adding atoms or molecules to the system (see the *fix pour*, *fix deposit*, and *fix gcmc* commands) or expect atoms or molecules to be lost (e.g. due to exiting the simulation box or via *fix evaporate*), then this option should be used to insure the temperature is correctly normalized.

Note: The *extra* and *dynamic* keywords should not be used as they are deprecated (March 2017) and will eventually be disabled. Instead, use the equivalent *extra/dof* and *dynamic/dof* keywords.

15.16.4 Restrictions

none

15.16.5 Related commands

compute

15.16.6 Default

The option defaults are extra/dof = 2 or 3 for 2d or 3d systems and dynamic/dof = no.

15.17 create_atoms command

15.17.1 Syntax

```
create_atoms type style args keyword values ...
```

- type = atom type (1-Ntypes) of atoms to create (offset for molecule creation)
- style = *box* or *region* or *single* or *random*

```
box args = none
region args = region-ID
  region-ID = particles will only be created if contained in the region
single args = x y z
  x,y,z = coordinates of a single particle (distance units)
random args = N seed region-ID
  N = number of particles to create
  seed = random # seed (positive integer)
  region-ID = create atoms within this region, use NULL for entire␣
↪simulation box
```

- zero or more keyword/value pairs may be appended
- keyword = *mol* or *basis* or *ratio* or *subset* or *remap* or *var* or *set* or *rotate* or *units*

```
*mol* value = template-ID seed
  template-ID = ID of molecule template specified in a separate :doc:`molecule
↪<molecule>` command
  seed = random # seed (positive integer)
*basis* values = M itype
  M = which basis atom
  itype = atom type (1-N) to assign to this basis atom
*ratio* values = frac seed
  frac = fraction of lattice sites (0 to 1) to populate randomly
  seed = random # seed (positive integer)
*subset* values = Nsubset seed
  Nsubset = # of lattice sites to populate randomly
  seed = random # seed (positive integer)
*remap* value = *yes* or *no*
*var* value = name = variable name to evaluate for test of atom creation
*set* values = dim name
  dim = *x* or *y* or *z*
  name = name of variable to set with x, y, or z atom position
*rotate* values = theta Rx Ry Rz
  theta = rotation angle for single molecule (degrees)
  Rx,Ry,Rz = rotation vector for single molecule
*units* value = *lattice* or *box*
  *lattice* = the geometry is defined in lattice units
  *box* = the geometry is defined in simulation box units
```

15.17.2 Examples

```
create_atoms 1 box
create_atoms 3 region regsphere basis 2 3
create_atoms 3 region regsphere basis 2 3 ratio 0.5 74637
create_atoms 3 single 0 0 5
create_atoms 1 box var v set x xpos set y ypos
```

15.17.3 Description

This command creates atoms (or molecules) on a lattice, or a single atom (or molecule), or a random collection of atoms (or molecules), as an alternative to reading in their coordinates explicitly via a *read_data* or *read_restart* command. A simulation box must already exist, which is typically created via the *create_box* command. Before using this command, a lattice must also be defined using the *lattice* command, unless you specify the *single* style with units = box or the *random* style. For the remainder of this doc page, a created atom or molecule is referred to as a "particle".

If created particles are individual atoms, they are assigned the specified atom *type*, though this can be altered via the *basis* keyword as discussed below. If molecules are being created, the type of each atom in the created molecule is specified in the file read by the *molecule* command, and those values are added to the specified atom *type*. E.g. if *type* = 2, and the file specifies atom types 1,2,3, then each created molecule will have atom types 3,4,5.

For the *box* style, the create_atoms command fills the entire simulation box with particles on the lattice. If your simulation box is periodic, you should insure its size is a multiple of the lattice spacings, to avoid unwanted atom overlaps at the box boundaries. If your box is periodic and a multiple of the lattice spacing in a particular dimension, LAMMPS is careful to put exactly one particle at the boundary (on either side of the box), not zero or two.

For the *region* style, a geometric volume is filled with particles on the lattice. This volume what is inside the simulation box and is also consistent with the region volume. See the *region* command for details. Note that a region can be specified so that its "volume" is either inside or outside a geometric boundary. Also note that if your region is the same size as a periodic simulation box (in some dimension), LAMMPS does not implement the same logic described above as for the *box* style, to insure exactly one particle at periodic boundaries. if this is what you desire, you should either use the *box* style, or tweak the region size to get precisely the particles you want.

For the *single* style, a single particle is added to the system at the specified coordinates. This can be useful for debugging purposes or to create a tiny system with a handful of particles at specified positions.

For the *random* style, N particles are added to the system at randomly generated coordinates, which can be useful for generating an amorphous system. The particles are created one by one using the specified random number *seed*, resulting in the same set of particles coordinates, independent of how many processors are being used in the simulation. If the *region-ID* argument is specified as NULL, then the created particles will be anywhere in the simulation box. If a *region-ID* is specified, a geometric volume is filled which is both inside the simulation box and is also consistent with the region volume. See the *region* command for details. Note that a region can be specified so that its "volume" is either inside or outside a geometric boundary.

Note: Particles generated by the *random* style will typically be highly overlapped which will cause many interatomic potentials to compute large energies and forces. Thus you should either perform an *energy minimization* or run dynamics with *fix nve/limit* to equilibrate such a system, before running normal dynamics.

Note that this command adds particles to those that already exist. This means it can be used to add particles to a system previously read in from a data or restart file. Or the create_atoms command can be used multiple times, to add multiple sets of particles to the simulation. For example, grain boundaries can be created, by interleaving create_atoms with *lattice* commands specifying different orientations. By using the create_atoms command in conjunction with the *delete_atoms* command, reasonably complex geometries can be created, or a protein can be solvated with a surrounding box of water molecules.

In all these cases, care should be taken to insure that new atoms do not overlap existing atoms inappropriately, especially if molecules are being added. The *delete_atoms* command can be used to remove overlapping atoms or molecules.

Note: You cannot use any of the styles explained above to create atoms that are outside the simulation box; they will just be ignored by LAMMPS. This is true even if you are using shrink-wrapped box boundaries, as specified by the *boundary* command. However, you can first use the *change_box* command to temporarily expand the box, then add atoms via create_atoms, then finally use change_box command again if needed to re-shrink-wrap the new atoms. See

the *change_box* doc page for an example of how to do this, using the create_atoms *single* style to insert a new atom outside the current simulation box.

Individual atoms are inserted by this command, unless the *mol* keyword is used. It specifies a *template-ID* previously defined using the *molecule* command, which reads a file that defines the molecule. The coordinates, atom types, charges, etc, as well as any bond/angle/etc and special neighbor information for the molecule can be specified in the molecule file. See the *molecule* command for details. The only settings required to be in this file are the coordinates and types of atoms in the molecule.

Using a lattice to add molecules, e.g. via the *box* or *region* or *single* styles, is exactly the same as adding atoms on lattice points, except that entire molecules are added at each point, i.e. on the point defined by each basis atom in the unit cell as it tiles the simulation box or region. This is done by placing the geometric center of the molecule at the lattice point, and giving the molecule a random orientation about the point. The random *seed* specified with the *mol* keyword is used for this operation, and the random numbers generated by each processor are different. This means the coordinates of individual atoms (in the molecules) will be different when running on different numbers of processors, unlike when atoms are being created in parallel.

Also note that because of the random rotations, it may be important to use a lattice with a large enough spacing that adjacent molecules will not overlap, regardless of their relative orientations.

Note: If the *create_box* command is used to create the simulation box, followed by the create_atoms command with its *mol* option for adding molecules, then you typically need to use the optional keywords allowed by the *create_box* command for extra bonds (angles,etc) or extra special neighbors. This is because by default, the *create_box* command sets up a non-molecular system which doesn't allow molecules to be added.

This is the meaning of the other allowed keywords.

The *basis* keyword is only used when atoms (not molecules) are being created. It specifies an atom type that will be assigned to specific basis atoms as they are created. See the *lattice* command for specifics on how basis atoms are defined for the unit cell of the lattice. By default, all created atoms are assigned the argument *type* as their atom type.

The *ratio* and *subset* keywords can be used in conjunction with the *box* or *region* styles to limit the total number of particles inserted. The lattice defines a set of *Nlatt* eligible sites for inserting particles, which may be limited by the *region* style or the *var* and *set* keywords. For the *ratio* keyword only the specified fraction of them (0 <= *frac* <= 1) will be assigned particles. For the *subset* keyword only the specified *Nsubset* of them will be assigned particles. In both cases the assigned lattice sites are chosen randomly. An iterative algorithm is used which insures the correct number of particles are inserted, in a perfectly random fashion. Which lattice sites are selected will change with the number of processors used.

The *remap* keyword only applies to the *single* style. If it is set to *yes*, then if the specified position is outside the simulation box, it will mapped back into the box, assuming the relevant dimensions are periodic. If it is set to *no*, no remapping is done and no particle is created if its position is outside the box.

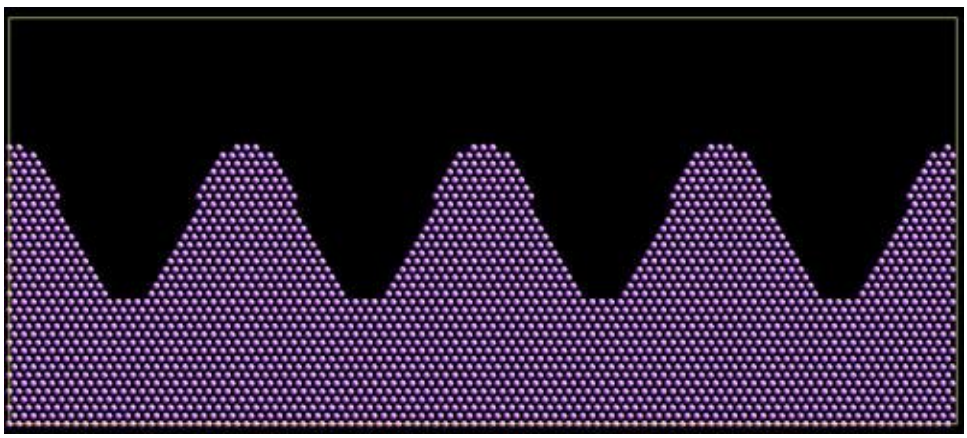
The *var* and *set* keywords can be used together to provide a criterion for accepting or rejecting the addition of an individual atom, based on its coordinates. The *name* specified for the *var* keyword is the name of an *equal-style variable* which should evaluate to a zero or non-zero value based on one or two or three variables which will store the x, y, or z coordinates of an atom (one variable per coordinate). If used, these other variables must be *internal-style variables* defined in the input script; their initial numeric value can be anything. They must be internal-style variables, because this command resets their values directly. The *set* keyword is used to identify the names of these other variables, one variable for the x-coordinate of a created atom, one for y, and one for z.

When an atom is created, its x,y,z coordinates become the values for any *set* variable that is defined. The *var* variable is then evaluated. If the returned value is 0.0, the atom is not created. If it is non-zero, the atom is created.

As an example, these commands can be used in a 2d simulation, to create a sinusoidal surface. Note that the surface is "rough" due to individual lattice points being "above" or "below" the mathematical expression for the sinusoidal curve. If a finer lattice were used, the sinusoid would appear to be "smoother". Also note the use of the "xlat" and "ylat" *thermo_style* keywords which converts lattice spacings to distance. Click on the image for a larger version.

```
dimension       2
variable        x equal 100
variable        y equal 25
lattice         hex 0.8442
region          box block 0 $x 0 $y -0.5 0.5
create_box      1 box

variable        xx internal 0.0
variable        yy internal 0.0
variable        v equal "(0.2*v_y*ylat * cos(v_xx/xlat * 2.0*PI*4.0/v_x) + 0.5*v_
↪y*ylat - v_yy) > 0.0"
create_atoms    1 box var v set x xx set y yy
write_dump      all atom sinusoid.lammpstrj
```



The *rotate* keyword allows specification of the orientation at which molecules are inserted. The axis of rotation is determined by the rotation vector (Rx,Ry,Rz) that goes through the insertion point. The specified *theta* determines the angle of rotation around that axis. Note that the direction of rotation for the atoms around the rotation axis is consistent with the right-hand rule: if your right-hand's thumb points along *R*, then your fingers wrap around the axis in the direction of rotation.

The *units* keyword determines the meaning of the distance units used to specify the coordinates of the one particle created by the *single* style. A *box* value selects standard distance units as defined by the *units* command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings.

Atom IDs are assigned to created atoms in the following way. The collection of created atoms are assigned consecutive IDs that start immediately following the largest atom ID existing before the create_atoms command was invoked. This is done by the processor's communicating the number of atoms they each own, the first processor numbering its atoms from 1 to N1, the second processor from N1+1 to N2, etc. Where N1 = number of atoms owned by the first processor, N2 = number owned by the second processor, etc. Thus when the same simulation is performed on different numbers of processors, there is no guarantee a particular created atom will be assigned the same ID in both simulations. If molecules are being created, molecule IDs are assigned to created molecules in a similar fashion.

Aside from their ID, atom type, and xyz position, other properties of created atoms are set to default values, depending on which quantities are defined by the chosen *atom style*. See the *atom style* command for more details. See the *set* and *velocity* commands for info on how to change these values.

- charge = 0.0

- dipole moment magnitude = 0.0
- diameter = 1.0
- shape = 0.0 0.0 0.0
- density = 1.0
- volume = 1.0
- velocity = 0.0 0.0 0.0
- angular velocity = 0.0 0.0 0.0
- angular momentum = 0.0 0.0 0.0
- quaternion = (1,0,0,0)
- bonds, angles, dihedrals, impropers = none

If molecules are being created, these defaults can be overridden by values specified in the file read by the *molecule* command. E.g. the file typically defines bonds (angles,etc) between atoms in the molecule, and can optionally define charges on each atom.

Note that the *sphere* atom style sets the default particle diameter to 1.0 as well as the density. This means the mass for the particle is not 1.0, but is PI/6 * diameter^3 = 0.5236.

Note that the *ellipsoid* atom style sets the default particle shape to (0.0 0.0 0.0) and the density to 1.0 which means it is a point particle, not an ellipsoid, and has a mass of 1.0.

Note that the *peri* style sets the default volume and density to 1.0 and thus also set the mass for the particle to 1.0.

The *set* command can be used to override many of these default settings.

15.17.4 Restrictions

An *atom_style* must be previously defined to use this command.

A rotation vector specified for a single molecule must be in the z-direction for a 2d model.

15.17.5 Related commands

lattice, *region*, *create_box*, *read_data*, *read_restart*

15.17.6 Default

The default for the *basis* keyword is that all created atoms are assigned the argument *type* as their atom type (when single atoms are being created). The other defaults are *remap* = no, *rotate* = random, and *units* = lattice.

15.18 create_bonds command

15.18.1 Syntax

```
create_bonds style args ... keyword value ...
```

- style = *many* or *single/bond* or *single/angle* or *single/dihedral*

```
many args = group-ID group2-ID btype rmin rmax
  group-ID = ID of first group
  group2-ID = ID of second group, bonds will be between atoms in the 2 groups
  btype = bond type of created bonds
  rmin = minimum distance between pair of atoms to bond together
  rmax = maximum distance between pair of atoms to bond together
single/bond args = btype batom1 batom2
  btype = bond type of new bond
  batom1,batom2 = atom IDs for two atoms in bond
single/angle args = atype aatom1 aatom2 aatom3
  atype = angle type of new angle
  aatom1,aatom2,aatom3 = atom IDs for three atoms in angle
single/dihedral args = dtype datom1 datom2 datom3 datom4
  dtype = dihedral type of new dihedral
  datom1,datom2,datom3,datom4 = atom IDs for four atoms in dihedral
single/improper args = itype iatom1 iatom2 iatom3 iatom4
  itype = improper type of new improper
  iatom1,iatom2,iatom3,iatom4 = atom IDs for four atoms in improper
```

- zero or more keyword/value pairs may be appended
- keyword = *special*

```
special value = yes or no
```

15.18.2 Examples

```
create_bonds many all all 1 1.0 1.2
create_bonds many surf solvent 3 2.0 2.4
create_bonds single/bond 1 1 2
create_bonds single/angle 5 52 98 107 special no
create_bonds single/dihedral 2 4 19 27 101
create_bonds single/improper 3 23 26 31 57
```

15.18.3 Description

Create bonds between pairs of atoms that meet a specified distance criteria. Or create a single bond, angle, dihedral or improper between 2, 3, or 4 specified atoms.

The new bond (angle, dihedral, improper) interactions will then be computed during a simulation by the bond (angle, dihedral, improper) potential defined by the *bond_style*, *bond_coeff*, *angle_style*, *angle_coeff*, *dihedral_style*, *dihedral_coeff*, *improper_style*, *improper_coeff* commands.

The *many* style is useful for adding bonds to a system, e.g. between nearest neighbors in a lattice of atoms, without having to enumerate all the bonds in the data file read by the *read_data* command.

The *single* styles are useful for adding bonds, angles, dihedrals, impropers to a system incrementally, then continuing a simulation.

Note that this command does not auto-create any angle, dihedral or improper interactions when a bond is added. Nor does it auto-create any bonds when an angle, dihedral or improper is added. Or auto-create any angles when a dihedral or improper is added. Thus the flexibility of this command is limited. It can be used several times to create different types of bond at different distances. But it cannot typically auto-create all the bonds or angles or dihedrals or impropers that would normally be defined in a data file for a complex system of molecules.

Note: If the system has no bonds (angles, dihedrals, impropers) to begin with, or if more bonds per atom are being added than currently exist, then you must insure that the number of bond types and the maximum number of bonds per atom are set to large enough values. And similarly for angles, dihedrals and impropers. Otherwise an error may occur when too many bonds (angles, dihedrals, impropers) are added to an atom. If the *read_data* command is used to define the system, these parameters can be set via the "bond types" and "extra bond per atom" fields in the header section of the data file. If the *create_box* command is used to define the system, these 2 parameters can be set via its optional "bond/types" and "extra/bond/per/atom" arguments. And similarly for angles, dihedrals and impropers. See the doc pages for these 2 commands for details.

The *many* style will create bonds between pairs of atoms I,J where I is in one of the two specified groups, and J is in the other. The two groups can be the same, e.g. group "all". The created bonds will be of bond type *btype*, where *btype* must be a value between 1 and the number of bond types defined.

For a bond to be created, an I,J pair of atoms must be a distance D apart such that *rmin* <= D <= *rmax*.

The following settings must have been made in an input script before this style is used:

- special_bonds weight for 1-2 interactions must be 0.0
- a *pair_style* must be defined
- no *kspace_style* defined
- minimum *pair_style* cutoff + *neighbor* skin >= *rmax*

These settings are required so that a neighbor list can be created to search for nearby atoms. Pairs of atoms that are already bonded cannot appear in the neighbor list, to avoid creation of duplicate bonds. The neighbor list for all atom type pairs must also extend to a distance that encompasses the *rmax* for new bonds to create.

An additional requirement for this style is that your system must be ready to perform a simulation. This means, for example, that all *pair_style* coefficients be set via the *pair_coeff* command. A *bond_style* command and all bond coefficients must also be set, even if no bonds exist before this command is invoked. This is because the building of neighbor list requires initialization and setup of a simulation, similar to what a *run* command would require.

Note that you can change any of these settings after this command executes, e.g. if you wish to use long-range Coulombic interactions via the *kspace_style* command for your subsequent simulation.

The *single/bond* style creates a single bond of type *btype* between two atoms with IDs *batom1* and *batom2*. *Btype* must be a value between 1 and the number of bond types defined.

The *single/angle* style creates a single angle of type *atype* between three atoms with IDs *aatom1*, *aatom2*, and *aatom3*. The ordering of the atoms is the same as in the *Angles* section of a data file read by the *read_data* command. I.e. the 3 atoms are ordered linearly within the angle; the central atom is *aatom2*. *Atype* must be a value between 1 and the number of angle types defined.

The *single/dihedral* style creates a single dihedral of type *dtype* between four atoms with IDs *datom1*, *datom2*, *datom3*, and *datom4*. The ordering of the atoms is the same as in the *Dihedrals* section of a data file read by the *read_data*

command. I.e. the 4 atoms are ordered linearly within the dihedral. *dtype* must be a value between 1 and the number of dihedral types defined.

The *single/improper* style creates a single improper of type *itype* between four atoms with IDs *iatom1*, *iatom2*, *iatom3*, and *iatom4*. The ordering of the atoms is the same as in the *Impropers* section of a data file read by the *read_data* command. I.e. the 4 atoms are ordered linearly within the improper. *itype* must be a value between 1 and the number of improper types defined.

The keyword *special* controls whether an internal list of special bonds is created after one or more bonds, or a single angle, dihedral or improper is added to the system.

The default value is *yes*. A value of *no* cannot be used with the *many* style.

This is an expensive operation since the bond topology for the system must be walked to find all 1-2, 1-3, 1-4 interactions to store in an internal list, which is used when pairwise interactions are weighted; see the *special_bonds* command for details.

Thus if you are adding a few bonds or a large list of angles all at the same time, by using this command repeatedly, it is more efficient to only trigger the internal list to be created once, after the last bond (or angle, or dihedral, or improper) is added:

```
create_bonds single/bond 5 52 98 special no
create_bonds single/bond 5 73 74 special no
...
create_bonds single/bond 5 17 386 special no
create_bonds single/bond 4 112 183 special yes
```

Note that you MUST insure the internal list is re-built after the last bond (angle, dihedral, improper) is added, before performing a simulation. Otherwise pairwise interactions will not be properly excluded or weighted. LAMMPS does NOT check that you have done this correctly.

15.18.4 Restrictions

This command cannot be used with molecular systems defined using molecule template files via the *molecule* and *atom_style template* commands.

15.18.5 Related commands

create_atoms, *delete_bonds*

15.18.6 Default

The keyword default is special = yes.

15.19 create_box command

15.19.1 Syntax

```
create_box N region-ID keyword value ...
```

- N = # of atom types to use in this simulation
- region-ID = ID of region to use as simulation domain
- zero or more keyword/value pairs may be appended
- keyword = *bond/types* or *angle/types* or *dihedral/types* or *improper/types* or *extra/bond/per/atom* or *extra/angle/per/atom* or *extra/dihedral/per/atom* or *extra/improper/per/atom*

  ```
  bond/types value = # of bond types
  angle/types value = # of angle types
  dihedral/types value = # of dihedral types
  improper/types value = # of improper types
  extra/bond/per/atom value = # of bonds per atom
  extra/angle/per/atom value = # of angles per atom
  extra/dihedral/per/atom value = # of dihedrals per atom
  extra/improper/per/atom value = # of impropers per atom
  extra/special/per/atom value = # of special neighbors per atom
  ```

15.19.2 Examples

```
create_box 2 mybox
create_box 2 mybox bond/types 2 extra/bond/per/atom 1
```

15.19.3 Description

This command creates a simulation box based on the specified region. Thus a *region* command must first be used to define a geometric domain. It also partitions the simulation box into a regular 3d grid of rectangular bricks, one per processor, based on the number of processors being used and the settings of the *processors* command. The partitioning can later be changed by the *balance* or *fix balance* commands.

The argument N is the number of atom types that will be used in the simulation.

If the region is not of style *prism*, then LAMMPS encloses the region (block, sphere, etc) with an axis-aligned orthogonal bounding box which becomes the simulation domain.

If the region is of style *prism*, LAMMPS creates a non-orthogonal simulation domain shaped as a parallelepiped with triclinic symmetry. As defined by the *region prism* command, the parallelepiped has its "origin" at (xlo,ylo,zlo) and is defined by 3 edge vectors starting from the origin given by A = (xhi-xlo,0,0); B = (xy,yhi-ylo,0); C = (xz,yz,zhi-zlo). *Xy,xz,yz* can be 0.0 or positive or negative values and are called "tilt factors" because they are the amount of displacement applied to faces of an originally orthogonal box to transform it into the parallelepiped.

By default, a *prism* region used with the create_box command must have tilt factors (xy,xz,yz) that do not skew the box more than half the distance of the parallel box length. For example, if xlo = 2 and xhi = 12, then the x box length is 10 and the xy tilt factor must be between -5 and 5. Similarly, both xz and yz must be between -(xhi-xlo)/2 and +(yhi-ylo)/2. Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = . . . , -15, -5, 5, 15, 25, . . . are all geometrically equivalent. If you wish to define a box with

tilt factors that exceed these limits, you can use the *box tilt* command, with a setting of *large*; a setting of *small* is the default.

See the *Howto triclinic* doc page for a geometric description of triclinic boxes, as defined by LAMMPS, and how to transform these parameters to and from other commonly used triclinic representations.

When a prism region is used, the simulation domain should normally be periodic in the dimension that the tilt is applied to, which is given by the second dimension of the tilt factor (e.g. y for xy tilt). This is so that pairs of atoms interacting across that boundary will have one of them shifted by the tilt factor. Periodicity is set by the *boundary* command. For example, if the xy tilt factor is non-zero, then the y dimension should be periodic. Similarly, the z dimension should be periodic if xz or yz is non-zero. LAMMPS does not require this periodicity, but you may lose atoms if this is not the case.

Also note that if your simulation will tilt the box, e.g. via the *fix deform* command, the simulation box must be setup to be triclinic, even if the tilt factors are initially 0.0. You can also change an orthogonal box to a triclinic box or vice versa by using the *change box* command with its *ortho* and *triclinic* options.

Note: If the system is non-periodic (in a dimension), then you should not make the lo/hi box dimensions (as defined in your *region* command) radically smaller/larger than the extent of the atoms you eventually plan to create, e.g. via the *create_atoms* command. For example, if your atoms extend from 0 to 50, you should not specify the box bounds as -10000 and 10000. This is because as described above, LAMMPS uses the specified box size to layout the 3d grid of processors. A huge (mostly empty) box will be sub-optimal for performance when using "fixed" boundary conditions (see the *boundary* command). When using "shrink-wrap" boundary conditions (see the *boundary* command), a huge (mostly empty) box may cause a parallel simulation to lose atoms the first time that LAMMPS shrink-wraps the box around the atoms.

The optional keywords can be used to create a system that allows for bond (angle, dihedral, improper) interactions, or for molecules with special 1-2,1-3,1-4 neighbors to be added later. These optional keywords serve the same purpose as the analogous keywords that can be used in a data file which are recognized by the *read_data* command when it sets up a system.

Note that if these keywords are not used, then the create_box command creates an atomic (non-molecular) simulation that does not allow bonds between pairs of atoms to be defined, or a *bond potential* to be specified, or for molecules with special neighbors to be added to the system by commands such as *create_atoms mol*, *fix deposit* or *fix pour*.

As an example, see the examples/deposit/in.deposit.molecule script, which deposits molecules onto a substrate. Initially there are no molecules in the system, but they are added later by the *fix deposit* command. The create_box command in the script uses the bond/types and extra/bond/per/atom keywords to allow this. If the added molecule contained more than 1 special bond (allowed by default), an extra/special/per/atom keyword would also need to be specified.

15.19.4 Restrictions

An *atom_style* and *region* must have been previously defined to use this command.

15.19.5 Related commands

read_data, *create_atoms*, *region*

Default: none

15.20 delete_atoms command

15.20.1 Syntax

```
delete_atoms style args keyword value ...
```

- style = *group* or *region* or *overlap* or *porosity*

```
group args = group-ID
region args = region-ID
overlap args = cutoff group1-ID group2-ID
  cutoff = delete one atom from pairs of atoms within the cutoff␣
↪(distance units)
  group1-ID = one atom in pair must be in this group
  group2-ID = other atom in pair must be in this group
porosity args = region-ID fraction seed
  region-ID = region within which to perform deletions
  fraction = delete this fraction of atoms
  seed = random number seed (positive integer)
```

- zero or more keyword/value pairs may be appended
- keyword = *compress* or *bond* or *mol*

```
compress value = no or yes
bond value = no or yes
mol value = no or yes
```

15.20.2 Examples

```
delete_atoms group edge
delete_atoms region sphere compress no
delete_atoms overlap 0.3 all all
delete_atoms overlap 0.5 solvent colloid
delete_atoms porosity cube 0.1 482793 bond yes
```

15.20.3 Description

Delete the specified atoms. This command can be used to carve out voids from a block of material or to delete created atoms that are too close to each other (e.g. at a grain boundary).

For style *group*, all atoms belonging to the group are deleted.

For style *region*, all atoms in the region volume are deleted. Additional atoms can be deleted if they are in a molecule for which one or more atoms were deleted within the region; see the *mol* keyword discussion below.

For style *overlap* pairs of atoms whose distance of separation is within the specified cutoff distance are searched for, and one of the 2 atoms is deleted. Only pairs where one of the two atoms is in the first group specified and the other atom is in the second group are considered. The atom that is in the first group is the one that is deleted.

Note that it is OK for the two group IDs to be the same (e.g. group *all*), or for some atoms to be members of both groups. In these cases, either atom in the pair may be deleted. Also note that if there are atoms which are members of both groups, the only guarantee is that at the end of the deletion operation, enough deletions will have occurred that no atom pairs within the cutoff will remain (subject to the group restriction). There is no guarantee that the minimum number of atoms will be deleted, or that the same atoms will be deleted when running on different numbers of processors.

For style *porosity* a specified *fraction* of atoms are deleted within the specified region. For example, if fraction is 0.1, then 10% of the atoms will be deleted. The atoms to delete are chosen randomly. There is no guarantee that the exact fraction of atoms will be deleted, or that the same atoms will be deleted when running on different numbers of processors.

If the *compress* keyword is set to *yes*, then after atoms are deleted, then atom IDs are re-assigned so that they run from 1 to the number of atoms in the system. Note that this is not done for molecular systems (see the *atom_style* command), regardless of the *compress* setting, since it would foul up the bond connectivity that has already been assigned. However, the *reset_ids* command can be used after this command to accomplish the same thing.

Note that the re-assignment of IDs is not really a compression, where gaps in atom IDs are removed by decrementing atom IDs that are larger. Instead the IDs for all atoms are erased, and new IDs are assigned so that the atoms owned by individual processors have consecutive IDs, as the *create_atoms* command explains.

A molecular system with fixed bonds, angles, dihedrals, or improper interactions, is one where the topology of the interactions is typically defined in the data file read by the *read_data* command, and where the interactions themselves are defined with the *bond_style*, *angle_style*, etc commands. If you delete atoms from such a system, you must be careful not to end up with bonded interactions that are stored by remaining atoms but which include deleted atoms. This will cause LAMMPS to generate a "missing atoms" error when the bonded interaction is computed. The *bond* and *mol* keywords offer two ways to do that.

It the *bond* keyword is set to *yes* then any bond or angle or dihedral or improper interaction that includes a deleted atom is also removed from the lists of such interactions stored by non-deleted atoms. Note that simply deleting interactions due to dangling bonds (e.g. at a surface) may result in a inaccurate or invalid model for the remaining atoms.

It the *mol* keyword is set to *yes*, then for every atom that is deleted, all other atoms in the same molecule (with the same molecule ID) will also be deleted. This is not done for atoms with molecule ID = 0, since such an ID is assumed to flag isolated atoms that are not part of molecules.

Note: The molecule deletion operation in invoked after all individual atoms have been deleted using the rules described above for each style. This means additional atoms may be deleted that are not in the group or region, that are not required by the overlap cutoff criterion, or that will create a higher fraction of porosity than was requested.

15.20.4 Restrictions

The *overlap* styles requires inter-processor communication to acquire ghost atoms and build a neighbor list. This means that your system must be ready to perform a simulation before using this command (force fields setup, atom masses set, etc). Since a neighbor list is used to find overlapping atom pairs, it also means that you must define a *pair style* with the minimum force cutoff distance between any pair of atoms types (plus the *neighbor* skin) >= the specified overlap cutoff.

If the *special_bonds* command is used with a setting of 0, then a pair of bonded atoms (1-2, 1-3, or 1-4) will not appear in the neighbor list, and thus will not be considered for deletion by the *overlap* styles. You probably don't want to be deleting one atom in a bonded pair anyway.

The *bond yes* option cannot be used with molecular systems defined using molecule template files via the *molecule* and *atom_style template* commands.

15.20.5 Related commands

create_atoms, *reset_ids*

15.20.6 Default

The option defaults are compress = yes, bond = no, mol = no.

15.21 delete_bonds command

15.21.1 Syntax

```
delete_bonds group-ID style arg keyword ...
```

- group-ID = group ID
- style = *multi* or *atom* or *bond* or *angle* or *dihedral* or *improper* or *stats*

  ```
  multi arg = none
  atom arg = an atom type or range of types (see below)
  bond arg = a bond type or range of types (see below)
  angle arg = an angle type or range of types (see below)
  dihedral arg = a dihedral type or range of types (see below)
  improper arg = an improper type or range of types (see below)
  stats arg = none
  ```
- zero or more keywords may be appended
- keyword = *any* or *undo* or *remove* or *special*

15.21.2 Examples

```
delete_bonds frozen multi remove
delete_bonds all atom 4 special
delete_bonds all bond 0*3 special
delete_bonds all stats
```

15.21.3 Description

Turn off (or on) molecular topology interactions, i.e. bonds, angles, dihedrals, impropers. This command is useful for deleting interactions that have been previously turned off by bond-breaking potentials. It is also useful for turning off topology interactions between frozen or rigid atoms. Pairwise interactions can be turned off via the *neigh_modify exclude* command. The *fix shake* command also effectively turns off certain bond and angle interactions.

For all styles, by default, an interaction is only turned off (or on) if all the atoms involved are in the specified group. See the *any* keyword to change the behavior.

Several of the styles (*atom*, *bond*, *angle*, *dihedral*, *improper*) take a *type* as an argument. The specified *type* should be an integer from 0 to N, where N is the number of relevant types (atom types, bond types, etc). A value of 0 is only relevant for style *bond*; see details below. In all cases, a wildcard asterisk can be used in place of or in conjunction with the *type* argument to specify a range of types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of types, then an asterisk with no numeric values means all types from 0 to N. A leading asterisk means all types from 0 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). Note that it is fine to include a type of 0 for non-bond styles; it will simply be ignored.

For style *multi* all bond, angle, dihedral, and improper interactions of any type, involving atoms in the group, are turned off.

Style *atom* is the same as style *multi* except that in addition, one or more of the atoms involved in the bond, angle, dihedral, or improper interaction must also be of the specified atom type.

For style *bond*, only bonds are candidates for turn-off, and the bond must also be of the specified type. Styles *angle*, *dihedral*, and *improper* are treated similarly.

For style *bond*, you can set the type to 0 to delete bonds that have been previously broken by a bond-breaking potential (which sets the bond type to 0 when a bond is broken); e.g. see the *bond_style quartic* command.

For style *stats* no interactions are turned off (or on); the status of all interactions in the specified group is simply reported. This is useful for diagnostic purposes if bonds have been turned off by a bond-breaking potential during a previous run.

The default behavior of the delete_bonds command is to turn off interactions by toggling their type to a negative value, but not to permanently remove the interaction. E.g. a bond_type of 2 is set to -2. The neighbor list creation routines will not include such an interaction in their interaction lists. The default is also to not alter the list of 1-2, 1-3, 1-4 neighbors computed by the *special_bonds* command and used to weight pairwise force and energy calculations. This means that pairwise computations will proceed as if the bond (or angle, etc) were still turned on.

Several keywords can be appended to the argument list to alter the default behaviors.

The *any* keyword changes the requirement that all atoms in the bond (angle, etc) must be in the specified group in order to turn-off the interaction. Instead, if any of the atoms in the interaction are in the specified group, it will be turned off (or on if the *undo* keyword is used).

The *undo* keyword inverts the delete_bonds command so that the specified bonds, angles, etc are turned on if they are currently turned off. This means a negative value is toggled to positive. For example, for style *angle*, if *type* is specified as 2, then all angles with current type = -2, are reset to type = 2. Note that the *fix shake* command also sets bond and angle types negative, so this option should not be used on those interactions.

The *remove* keyword is invoked at the end of the delete_bonds operation. It causes turned-off bonds (angles, etc) to be removed from each atom's data structure and then adjusts the global bond (angle, etc) counts accordingly. Removal is a permanent change; removed bonds cannot be turned back on via the *undo* keyword. Removal does not alter the pairwise 1-2, 1-3, 1-4 weighting list.

The *special* keyword is invoked at the end of the delete_bonds operation, after (optional) removal. It re-computes the pairwise 1-2, 1-3, 1-4 weighting list. The weighting list computation treats turned-off bonds the same as turned-on. Thus, turned-off bonds must be removed if you wish to change the weighting list.

Note that the choice of *remove* and *special* options affects how 1-2, 1-3, 1-4 pairwise interactions will be computed across bonds that have been modified by the delete_bonds command.

15.21.4 Restrictions

This command requires inter-processor communication to acquire ghost atoms, to coordinate the deleting of bonds, angles, etc between atoms shared by multiple processors. This means that your system must be ready to perform a simulation before using this command (force fields setup, atom masses set, etc). Just as would be needed to run dynamics, the force field you define should define a cutoff (e.g. through a *pair_style* command) which is long enough for a processor to acquire the ghost atoms its needs to compute bond, angle, etc interactions.

If deleted bonds (angles, etc) are removed but the 1-2, 1-3, 1-4 weighting list is not re-computed, this can cause a later *fix shake* command to fail due to an atom's bonds being inconsistent with the weighting list. This should only happen if the group used in the fix command includes both atoms in the bond, in which case you probably should be recomputing the weighting list.

15.21.5 Related commands

neigh_modify exclude, *special_bonds*, *fix shake*

Default: none

15.22 dielectric command

15.22.1 Syntax

```
dielectric value
```

- value = dielectric constant

15.22.2 Examples

```
dielectric 2.0
```

15.22.3 Description

Set the dielectric constant for Coulombic interactions (pairwise and long-range) to this value. The constant is unitless, since it is used to reduce the strength of the interactions. The value is used in the denominator of the formulas for Coulombic interactions - e.g. a value of 4.0 reduces the Coulombic interactions to 25% of their default strength. See the *pair_style* command for more details.

15.22.4 Restrictions

none

15.22.5 Related commands

pair_style

15.22.6 Default

```
dielectric 1.0
```

15.23 dihedral_coeff command

15.23.1 Syntax

```
dihedral_coeff N args
```

- N = dihedral type (see asterisk form below)
- args = coefficients for one or more dihedral types

15.23.2 Examples

```
dihedral_coeff 1 80.0 1 3
dihedral_coeff * 80.0 1 3 0.5
dihedral_coeff 2* 80.0 1 3 0.5
```

15.23.3 Description

Specify the dihedral force field coefficients for one or more dihedral types. The number and meaning of the coefficients depends on the dihedral style. Dihedral coefficients can also be set in the data file read by the *read_data* command or in a restart file.

N can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to set the coefficients for multiple dihedral types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of dihedral types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

Note that using a dihedral_coeff command can override a previous setting for the same dihedral type. For example, these commands set the coeffs for all dihedral types, then overwrite the coeffs for just dihedral type 2:

```
dihedral_coeff * 80.0 1 3
dihedral_coeff 2 200.0 1 3
```

A line in a data file that specifies dihedral coefficients uses the exact same format as the arguments of the dihedral_coeff command in an input script, except that wild-card asterisks should not be used since coefficients for all N types must be listed in the file. For example, under the "Dihedral Coeffs" section of a data file, the line that corresponds to the 1st example above would be listed as

```
1 80.0 1 3
```

The *dihedral_style class2* is an exception to this rule, in that an additional argument is used in the input script to allow specification of the cross-term coefficients. See its doc page for details.

Note: When comparing the formulas and coefficients for various LAMMPS dihedral styles with dihedral equations defined by other force fields, note that some force field implementations divide/multiply the energy prefactor K by the multiple number of torsions that contain the J-K bond in an I-J-K-L torsion. LAMMPS does not do this, i.e. the listed dihedral equation applies to each individual dihedral. Thus you need to define K appropriately to account for this difference if necessary.

The list of all dihedral styles defined in LAMMPS is given on the *dihedral_style* doc page. They are also listed in more compact form on the *Commands dihedral* doc page.

On either of those pages, click on the style to display the formula it computes and its coefficients as specified by the associated dihedral_coeff command.

15.23.4 Restrictions

This command must come after the simulation box is defined by a *read_data*, *read_restart*, or *create_box* command.

A dihedral style must be defined before any dihedral coefficients are set, either in the input script or in a data file.

15.23.5 Related commands

dihedral_style

Default: none

15.24 dihedral_style command

15.24.1 Syntax

```
dihedral_style style
```

- style = *none* or *hybrid* or *charmm* or *class2* or *harmonic* or *helix* or *multi/harmonic* or *opls*

15.24.2 Examples

```
dihedral_style harmonic
dihedral_style multi/harmonic
dihedral_style hybrid harmonic charmm
```

15.24.3 Description

Set the formula(s) LAMMPS uses to compute dihedral interactions between quadruplets of atoms, which remain in force for the duration of the simulation. The list of dihedral quadruplets is read in by a *read_data* or *read_restart* command from a data or restart file.

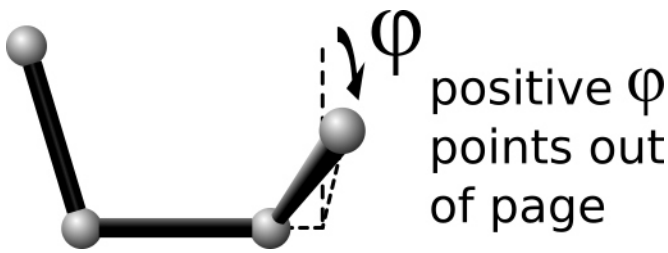
Hybrid models where dihedrals are computed using different dihedral potentials can be setup using the *hybrid* dihedral style.

The coefficients associated with a dihedral style can be specified in a data or restart file or via the *dihedral_coeff* command.

All dihedral potentials store their coefficient data in binary restart files which means dihedral_style and *dihedral_coeff* commands do not need to be re-specified in an input script that restarts a simulation. See the *read_restart* command for details on how to do this. The one exception is that dihedral_style *hybrid* only stores the list of sub-styles in the restart file; dihedral coefficients need to be re-specified.

Note: When both a dihedral and pair style is defined, the *special_bonds* command often needs to be used to turn off (or weight) the pairwise interaction that would otherwise exist between 4 bonded atoms.

In the formulas listed for each dihedral style, *phi* is the torsional angle defined by the quadruplet of atoms. This angle has a sign convention as shown in this diagram:



where the I,J,K,L ordering of the 4 atoms that define the dihedral is from left to right.

This sign convention effects several of the dihedral styles listed below (e.g. charmm, helix) in the sense that the energy formula depends on the sign of phi, which may be reflected in the value of the coefficients you specify.

Note: When comparing the formulas and coefficients for various LAMMPS dihedral styles with dihedral equations defined by other force fields, note that some force field implementations divide/multiply the energy prefactor *K* by the multiple number of torsions that contain the J-K bond in an I-J-K-L torsion. LAMMPS does not do this, i.e. the listed dihedral equation applies to each individual dihedral. Thus you need to define *K* appropriately via the *dihedral_coeff* command to account for this difference if necessary.

Here is an alphabetic list of dihedral styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated *dihedral_coeff* command.

Click on the style to display the formula it computes, any additional arguments specified in the dihedral_style command, and coefficients specified by the associated *dihedral_coeff* command.

There are also additional accelerated pair styles included in the LAMMPS distribution for faster performance on CPUs, GPUs, and KNLs. The individual style names on the *Commands dihedral* doc page are followed by one or more of (g,i,k,o,t) to indicate which accelerated styles exist.

- *none* - turn off dihedral interactions
- *zero* - topology but no interactions

- *hybrid* - define multiple styles of dihedral interactions
- *charmm* - CHARMM dihedral
- *charmmfsw* - CHARMM dihedral with force switching
- *class2* - COMPASS (class 2) dihedral
- *cosine/shift/exp* - dihedral with exponential in spring constant
- *fourier* - dihedral with multiple cosine terms
- *harmonic* - harmonic dihedral
- *helix* - helix dihedral
- *multi/harmonic* - dihedral with 5 harmonic terms
- *nharmonic* - same as multi-harmonic with N terms
- *opls* - OPLS dihedral
- *quadratic* - dihedral with quadratic term in angle
- *spherical* - dihedral which includes angle terms to avoid singularities
- *table* - tabulated dihedral
- *table/cut* - tabulated dihedral with analytic cutoff

15.24.4 Restrictions

Dihedral styles can only be set for atom styles that allow dihedrals to be defined.

Most dihedral styles are part of the MOLECULE package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info. The doc pages for individual dihedral potentials tell if it is part of a package.

15.24.5 Related commands

dihedral_coeff

15.24.6 Default

dihedral_style none

15.25 dimension command

15.25.1 Syntax

```
dimension N
```

- N = 2 or 3

15.25.2 Examples

```
dimension 2
```

15.25.3 Description

Set the dimensionality of the simulation. By default LAMMPS runs 3d simulations. To run a 2d simulation, this command should be used prior to setting up a simulation box via the *create_box* or *read_data* commands. Restart files also store this setting.

See the discussion on the *Howto 2d* doc page for additional instructions on how to run 2d simulations.

Note: Some models in LAMMPS treat particles as finite-size spheres or ellipsoids, as opposed to point particles. In 2d, the particles will still be spheres or ellipsoids, not circular disks or ellipses, meaning their moment of inertia will be the same as in 3d.

15.25.4 Restrictions

This command must be used before the simulation box is defined by a *read_data* or *create_box* command.

15.25.5 Related commands

fix enforce2d

15.25.6 Default

```
dimension 3
```

15.26 displace_atoms command

15.26.1 Syntax

```
displace_atoms group-ID style args keyword value ...
```

- group-ID = ID of group of atoms to displace
- style = *move* or *ramp* or *random* or *rotate*

```
move args = delx dely delz
  delx,dely,delz = distance to displace in each dimension (distance units)
  any of delx,dely,delz can be a variable (see below)
ramp args = ddim dlo dhi dim clo chi
  ddim = x or y or z
  dlo,dhi = displacement distance between dlo and dhi (distance units)
  dim = x or y or z
  clo,chi = lower and upper bound of domain to displace (distance units)
random args = dx dy dz seed
```

```
  dx,dy,dz = random displacement magnitude in each dimension (distance␣
↪units)
  seed = random # seed (positive integer)
rotate args = Px Py Pz Rx Ry Rz theta
  Px,Py,Pz = origin point of axis of rotation (distance units)
  Rx,Ry,Rz = axis of rotation vector
  theta = angle of rotation (degrees)
```

- zero or more keyword/value pairs may be appended

```
keyword = units
  value = box or lattice
```

15.26.2 Examples

```
displace_atoms top move 0 -5 0 units box
displace_atoms flow ramp x 0.0 5.0 y 2.0 20.5
```

15.26.3 Description

Displace a group of atoms. This can be used to move atoms a large distance before beginning a simulation or to randomize atoms initially on a lattice. For example, in a shear simulation, an initial strain can be imposed on the system. Or two groups of atoms can be brought into closer proximity.

The *move* style displaces the group of atoms by the specified 3d displacement vector. Any of the 3 quantities defining the vector components can be specified as an equal-style or atom-style *variable*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated, and its value(s) used for the displacement(s). The scale factor implied by the *units* keyword will also be applied to the variable result.

Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates or per-atom values read from a file. Note that if the variable references other *compute* or *fix* commands, those values must be up-to-date for the current timestep. See the "Variable Accuracy" section of the *variable* doc page for more details.

The *ramp* style displaces atoms a variable amount in one dimension depending on the atom's coordinate in a (possibly) different dimension. For example, the second example command displaces atoms in the x-direction an amount between 0.0 and 5.0 distance units. Each atom's displacement depends on the fractional distance its y coordinate is between 2.0 and 20.5. Atoms with y-coordinates outside those bounds will be moved the minimum (0.0) or maximum (5.0) amount.

The *random* style independently moves each atom in the group by a random displacement, uniformly sampled from a value between -dx and +dx in the x dimension, and similarly for y and z. Random numbers are used in such a way that the displacement of a particular atom is the same, regardless of how many processors are being used.

The *rotate* style rotates each atom in the group by the angle *theta* around a rotation axis R = (Rx,Ry,Rz) that goes through a point P = (Px,Py,Pz). The direction of rotation for the atoms around the rotation axis is consistent with the right-hand rule: if your right-hand thumb points along R, then your fingers wrap around the axis in the direction of positive theta.

If the defined *atom_style* assigns an orientation to each atom (*atom styles* ellipsoid, line, tri, body), then that property is also updated appropriately to correspond to the atom's rotation.

Distance units for displacements and the origin point of the *rotate* style are determined by the setting of *box* or *lattice* for the *units* keyword. *Box* means distance units as defined by the *units* command - e.g. Angstroms for *real* units.

Lattice means distance units are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacing.

Note: Care should be taken not to move atoms on top of other atoms. After the move, atoms are remapped into the periodic simulation box if needed, and any shrink-wrap boundary conditions (see the *boundary* command) are enforced which may change the box size. Other than this effect, this command does not change the size or shape of the simulation box. See the *change_box* command if that effect is desired.

Note: Atoms can be moved arbitrarily long distances by this command. If the simulation box is non-periodic and shrink-wrapped (see the *boundary* command), this can change its size or shape. This is not a problem, except that the mapping of processors to the simulation box is not changed by this command from its initial 3d configuration; see the *processors* command. Thus, if the box size/shape changes dramatically, the mapping of processors to the simulation box may not end up as optimal as the initial mapping attempted to be.

15.26.4 Restrictions

For a 2d simulation, only rotations around the a vector parallel to the z-axis are allowed.

15.26.5 Related commands

lattice, *change_box*, *fix move*

15.26.6 Default

The option defaults are units = lattice.

15.27 dump command

15.28 dump vtk command

15.29 dump h5md command

15.30 dump molfile command

15.31 dump netcdf command

15.32 dump image command

15.33 dump movie command

15.34 dump atom/adios command

15.35 dump custom/adios command

15.35.1 Syntax

```
dump ID group-ID style N file args
```

- ID = user-assigned name for the dump
- group-ID = ID of the group of atoms to be dumped
- style = *atom* or *atom/gz* or *atom/mpiio* or *cfg* or *cfg/gz* or *cfg/mpiio* or *custom* or *custom/gz* or *custom/mpiio* or *dcd* or *h5md* or *image* or *local* or *local/gz* or *molfile* or *movie* or *netcdf* or *netcdf/mpiio* or *vtk* or *xtc* or *xyz* or *xyz/gz* or *xyz/mpiio*
- N = dump every this many timesteps
- file = name of file to write dump info to
- args = list of arguments for a particular style

```
atom args = none
atom/gz args = none
atom/mpiio args = none
atom/adios args = none,  discussed on dump atom/adios doc page
cfg args = same as custom args, see below
cfg/gz args = same as custom args, see below
cfg/mpiio args = same as custom args, see below
custom, custom/gz, custom/mpiio args = see below
custom/adios args = same as custom args, discussed on dump custom/adios␣
↪doc page
dcd args = none
h5md args = discussed on dump h5md doc page
image args = discussed on dump image doc page
```

```
local args = see below
molfile args = discussed on dump molfile doc page
movie args = discussed on dump image doc page
netcdf args = discussed on dump netcdf doc page
netcdf/mpiio args = discussed on dump netcdf doc page
vtk args = same as custom args, see below, also dump vtk doc page
xtc args = none
xyz args = none
xyz/gz args = none
xyz/mpiio args = none
```

- *custom* or *custom/gz* or *custom/mpiio* or *netcdf* or *netcdf/mpiio* args = list of atom attributes

```
possible attributes = id, mol, proc, procp1, type, element, mass,
                      x, y, z, xs, ys, zs, xu, yu, zu,
                      xsu, ysu, zsu, ix, iy, iz,
                      vx, vy, vz, fx, fy, fz,
                      q, mux, muy, muz, mu,
                      radius, diameter, omegax, omegay, omegaz,
                      angmomx, angmomy, angmomz, tqx, tqy, tqz,
                      c_ID, c_ID[N], f_ID, f_ID[N], v_name
```

```
id = atom ID
mol = molecule ID
proc = ID of processor that owns atom
procp1 = ID+1 of processor that owns atom
type = atom type
element = name of atom element, as defined by dump_modify command
mass = atom mass
x,y,z = unscaled atom coordinates
xs,ys,zs = scaled atom coordinates
xu,yu,zu = unwrapped atom coordinates
xsu,ysu,zsu = scaled unwrapped atom coordinates
ix,iy,iz = box image that the atom is in
vx,vy,vz = atom velocities
fx,fy,fz = forces on atoms
q = atom charge
mux,muy,muz = orientation of dipole moment of atom
mu = magnitude of dipole moment of atom
radius,diameter = radius,diameter of spherical particle
omegax,omegay,omegaz = angular velocity of spherical particle
angmomx,angmomy,angmomz = angular momentum of aspherical particle
tqx,tqy,tqz = torque on finite-size particles
c_ID = per-atom vector calculated by a compute with ID
c_ID[I] = Ith column of per-atom array calculated by a compute with ID, I␣
↪can include wildcard (see below)
f_ID = per-atom vector calculated by a fix with ID
f_ID[I] = Ith column of per-atom array calculated by a fix with ID, I can␣
↪include wildcard (see below)
v_name = per-atom vector calculated by an atom-style variable with name
d_name = per-atom floating point vector with name, managed by fix␣
↪property/atom
i_name = per-atom integer vector with name, managed by fix property/atom
```

- *local* args = list of local attributes

```
possible attributes = index, c_ID, c_ID[I], f_ID, f_ID[I]
  index = enumeration of local values
  c_ID = local vector calculated by a compute with ID
  c_ID[I] = Ith column of local array calculated by a compute with ID, I can␣
↪include wildcard (see below)
  f_ID = local vector calculated by a fix with ID
  f_ID[I] = Ith column of local array calculated by a fix with ID, I can include␣
↪wildcard (see below)
```

15.35.2 Examples

```
dump myDump all atom 100 dump.atom
dump myDump all atom/mpiio 100 dump.atom.mpiio
dump myDump all atom/gz 100 dump.atom.gz
dump 2 subgroup atom 50 dump.run.bin
dump 2 subgroup atom 50 dump.run.mpiio.bin
dump 4a all custom 100 dump.myforce.* id type x y vx fx
dump 4b flow custom 100 dump.%.myforce id type c_myF[3] v_ke
dump 4b flow custom 100 dump.%.myforce id type c_myF[*] v_ke
dump 2 inner cfg 10 dump.snap.*.cfg mass type xs ys zs vx vy vz
dump snap all cfg 100 dump.config.*.cfg mass type xs ys zs id type c_Stress[2]
dump 1 all xtc 1000 file.xtc
```

15.35.3 Description

Dump a snapshot of atom quantities to one or more files every N timesteps in one of several styles. The *image* and *movie* styles are the exception: the *image* style renders a JPG, PNG, or PPM image file of the atom configuration every N timesteps while the *movie* style combines and compresses them into a movie file; both are discussed in detail on the *dump image* doc page. The timesteps on which dump output is written can also be controlled by a variable. See the *dump_modify every* command.

Only information for atoms in the specified group is dumped. The *dump_modify thresh and region and refresh* commands can also alter what atoms are included. Not all styles support these options; see details on the *dump_modify* doc page.

As described below, the filename determines the kind of output (text or binary or gzipped, one big file or one per timestep, one big file or multiple smaller files).

Note: Because periodic boundary conditions are enforced only on timesteps when neighbor lists are rebuilt, the coordinates of an atom written to a dump file may be slightly outside the simulation box. Re-neighbor timesteps will not typically coincide with the timesteps dump snapshots are written. See the *dump_modify pbc* command if you with to force coordinates to be strictly inside the simulation box.

Note: Unless the *dump_modify sort* option is invoked, the lines of atom information written to dump files (typically one line per atom) will be in an indeterminate order for each snapshot. This is even true when running on a single processor, if the *atom_modify sort* option is on, which it is by default. In this case atoms are re-ordered periodically during a simulation, due to spatial sorting. It is also true when running in parallel, because data for a single snapshot is collected from multiple processors, each of which owns a subset of the atoms.

For the *atom*, *custom*, *cfg*, and *local* styles, sorting is off by default. For the *dcd*, *xtc*, *xyz*, and *molfile* styles, sorting by atom ID is on by default. See the *dump_modify* doc page for details.

The *atom/gz*, *cfg/gz*, *custom/gz*, and *xyz/gz* styles are identical in command syntax to the corresponding styles without "gz", however, they generate compressed files using the zlib library. Thus the filename suffix ".gz" is mandatory. This is an alternative approach to writing compressed files via a pipe, as done by the regular dump styles, which may be required on clusters where the interface to the high-speed network disallows using the fork() library call (which is needed for a pipe). For the remainder of this doc page, you should thus consider the *atom* and *atom/gz* styles (etc) to be inter-changeable, with the exception of the required filename suffix.

As explained below, the *atom/mpiio*, *cfg/mpiio*, *custom/mpiio*, and *xyz/mpiio* styles are identical in command syntax and in the format of the dump files they create, to the corresponding styles without "mpiio", except the single dump file they produce is written in parallel via the MPI-IO library. For the remainder of this doc page, you should thus consider the *atom* and *atom/mpiio* styles (etc) to be inter-changeable. The one exception is how the filename is specified for the MPI-IO styles, as explained below.

The precision of values output to text-based dump files can be controlled by the *dump_modify format* command and its options.

The *style* keyword determines what atom quantities are written to the file and in what format. Settings made via the *dump_modify* command can also alter the format of individual values and the file itself.

The *atom*, *local*, and *custom* styles create files in a simple text format that is self-explanatory when viewing a dump file. Some of the LAMMPS post-processing tools described on the *Tools* doc page, including Pizza.py, work with this format, as does the *rerun* command.

For post-processing purposes the *atom*, *local*, and *custom* text files are self-describing in the following sense.

The dimensions of the simulation box are included in each snapshot. For an orthogonal simulation box this information is formatted as:

```
ITEM: BOX BOUNDS xx yy zz
xlo xhi
ylo yhi
zlo zhi
```

where xlo,xhi are the maximum extents of the simulation box in the x-dimension, and similarly for y and z. The "xx yy zz" represent 6 characters that encode the style of boundary for each of the 6 simulation box boundaries (xlo,xhi and ylo,yhi and zlo,zhi). Each of the 6 characters is either p = periodic, f = fixed, s = shrink wrap, or m = shrink wrapped with a minimum value. See the *boundary* command for details.

For triclinic simulation boxes (non-orthogonal), an orthogonal bounding box which encloses the triclinic simulation box is output, along with the 3 tilt factors (xy, xz, yz) of the triclinic box, formatted as follows:

```
ITEM: BOX BOUNDS xy xz yz xx yy zz
xlo_bound xhi_bound xy
ylo_bound yhi_bound xz
zlo_bound zhi_bound yz
```

The presence of the text "xy xz yz" in the ITEM line indicates that the 3 tilt factors will be included on each of the 3 following lines. This bounding box is convenient for many visualization programs. The meaning of the 6 character flags for "xx yy zz" is the same as above.

Note that the first two numbers on each line are now xlo_bound instead of xlo, etc, since they represent a bounding box. See the *Howto triclinic* doc page for a geometric description of triclinic boxes, as defined by LAMMPS, simple formulas for how the 6 bounding box extents (xlo_bound,xhi_bound,etc) are calculated from the triclinic parameters, and how to transform those parameters to and from other commonly used triclinic representations.

The "ITEM: ATOMS" line in each snapshot lists column descriptors for the per-atom lines that follow. For example, the descriptors would be "id type xs ys zs" for the default *atom* style, and would be the atom attributes you specify in the dump command for the *custom* style.

For style *atom*, atom coordinates are written to the file, along with the atom ID and atom type. By default, atom coords are written in a scaled format (from 0 to 1). I.e. an x value of 0.25 means the atom is at a location 1/4 of the distance from xlo to xhi of the box boundaries. The format can be changed to unscaled coords via the *dump_modify* settings. Image flags can also be added for each atom via dump_modify.

Style *custom* allows you to specify a list of atom attributes to be written to the dump file for each atom. Possible attributes are listed above and will appear in the order specified. You cannot specify a quantity that is not defined for a particular simulation - such as *q* for atom style *bond*, since that atom style doesn't assign charges. Dumps occur at the very end of a timestep, so atom attributes will include effects due to fixes that are applied during the timestep. An explanation of the possible dump custom attributes is given below.

For style *local*, local output generated by *computes* and *fixes* is used to generate lines of output that is written to the dump file. This local data is typically calculated by each processor based on the atoms it owns, but there may be zero or more entities per atom, e.g. a list of bond distances. An explanation of the possible dump local attributes is given below. Note that by using input from the *compute property/local* command with dump local, it is possible to generate information on bonds, angles, etc that can be cut and pasted directly into a data file read by the *read_data* command.

Style *cfg* has the same command syntax as style *custom* and writes extended CFG format files, as used by the AtomEye visualization package. Since the extended CFG format uses a single snapshot of the system per file, a wildcard "*" must be included in the filename, as discussed below. The list of atom attributes for style *cfg* must begin with either "mass type xs ys zs" or "mass type xsu ysu zsu" since these quantities are needed to write the CFG files in the appropriate format (though the "mass" and "type" fields do not appear explicitly in the file). Any remaining attributes will be stored as "auxiliary properties" in the CFG files. Note that you will typically want to use the *dump_modify element* command with CFG-formatted files, to associate element names with atom types, so that AtomEye can render atoms appropriately. When unwrapped coordinates *xsu*, *ysu*, and *zsu* are requested, the nominal AtomEye periodic cell dimensions are expanded by a large factor UNWRAPEXPAND = 10.0, which ensures atoms that are displayed correctly for up to UNWRAPEXPAND/2 periodic boundary crossings in any direction. Beyond this, AtomEye will rewrap the unwrapped coordinates. The expansion causes the atoms to be drawn farther away from the viewer, but it is easy to zoom the atoms closer, and the interatomic distances are unaffected.

The *dcd* style writes DCD files, a standard atomic trajectory format used by the CHARMM, NAMD, and XPlor molecular dynamics packages. DCD files are binary and thus may not be portable to different machines. The number of atoms per snapshot cannot change with the *dcd* style. The *unwrap* option of the *dump_modify* command allows DCD coordinates to be written "unwrapped" by the image flags for each atom. Unwrapped means that if the atom has passed through a periodic boundary one or more times, the value is printed for what the coordinate would be if it had not been wrapped back into the periodic box. Note that these coordinates may thus be far outside the box size stored with the snapshot.

The *xtc* style writes XTC files, a compressed trajectory format used by the GROMACS molecular dynamics package, and described here. The precision used in XTC files can be adjusted via the *dump_modify* command. The default value of 1000 means that coordinates are stored to 1/1000 nanometer accuracy. XTC files are portable binary files written in the NFS XDR data format, so that any machine which supports XDR should be able to read them. The number of atoms per snapshot cannot change with the *xtc* style. The *unwrap* option of the *dump_modify* command allows XTC coordinates to be written "unwrapped" by the image flags for each atom. Unwrapped means that if the atom has passed through a periodic boundary one or more times, the value is printed for what the coordinate would be if it had not been wrapped back into the periodic box. Note that these coordinates may thus be far outside the box size stored with the snapshot.

The *xyz* style writes XYZ files, which is a simple text-based coordinate format that many codes can read. Specifically it has a line with the number of atoms, then a comment line that is usually ignored followed by one line per atom with the atom type and the x-, y-, and z-coordinate of that atom. You can use the *dump_modify element* option to change the output from using the (numerical) atom type to an element name (or some other label). This will help many visualization programs to guess bonds and colors.

Note that *atom*, *custom*, *dcd*, *xtc*, and *xyz* style dump files can be read directly by VMD, a popular molecular viewing program.

Dumps are performed on timesteps that are a multiple of N (including timestep 0) and on the last timestep of a minimization if the minimization converges. Note that this means a dump will not be performed on the initial timestep after the dump command is invoked, if the current timestep is not a multiple of N. This behavior can be changed via the *dump_modify first* command, which can also be useful if the dump command is invoked after a minimization ended on an arbitrary timestep. N can be changed between runs by using the *dump_modify every* command (not allowed for *dcd* style). The *dump_modify every* command also allows a variable to be used to determine the sequence of timesteps on which dump files are written. In this mode a dump on the first timestep of a run will also not be written unless the *dump_modify first* command is used.

The specified filename determines how the dump file(s) is written. The default is to write one large text file, which is opened when the dump command is invoked and closed when an *undump* command is used or when LAMMPS exits. For the *dcd* and *xtc* styles, this is a single large binary file.

Dump filenames can contain two wildcard characters. If a "*" character appears in the filename, then one file per snapshot is written and the "*" character is replaced with the timestep value. For example, tmp.dump.* becomes tmp.dump.0, tmp.dump.10000, tmp.dump.20000, etc. This option is not available for the *dcd* and *xtc* styles. Note that the *dump_modify pad* command can be used to insure all timestep numbers are the same length (e.g. 00010), which can make it easier to read a series of dump files in order with some post-processing tools.

If a "%" character appears in the filename, then each of P processors writes a portion of the dump file, and the "%" character is replaced with the processor ID from 0 to P-1. For example, tmp.dump.% becomes tmp.dump.0, tmp.dump.1, ... tmp.dump.P-1, etc. This creates smaller files and can be a fast mode of output on parallel machines that support parallel I/O for output. This option is not available for the *dcd*, *xtc*, and *xyz* styles.

By default, P = the number of processors meaning one file per processor, but P can be set to a smaller value via the *nfile* or *fileper* keywords of the *dump_modify* command. These options can be the most efficient way of writing out dump files when running on large numbers of processors.

Note that using the "*" and "%" characters together can produce a large number of small dump files!

For the *atom/mpiio*, *cfg/mpiio*, *custom/mpiio*, and *xyz/mpiio* styles, a single dump file is written in parallel via the MPI-IO library, which is part of the MPI standard for versions 2.0 and above. Using MPI-IO requires two steps. First, build LAMMPS with its MPIIO package installed, e.g.

```
make yes-mpiio    # installs the MPIIO package
make mpi          # build LAMMPS for your platform
```

Second, use a dump filename which contains ".mpiio". Note that it does not have to end in ".mpiio", just contain those characters. Unlike MPI-IO restart files, which must be both written and read using MPI-IO, the dump files produced by these MPI-IO styles are identical in format to the files produced by their non-MPI-IO style counterparts. This means you can write a dump file using MPI-IO and use the *read_dump* command or perform other post-processing, just as if the dump file was not written using MPI-IO.

Note that MPI-IO dump files are one large file which all processors write to. You thus cannot use the "%" wildcard character described above in the filename since that specifies generation of multiple files. You can use the ".bin" suffix described below in an MPI-IO dump file; again this file will be written in parallel and have the same binary format as if it were written without MPI-IO.

If the filename ends with ".bin", the dump file (or files, if "*" or "%" is also used) is written in binary format. A binary dump file will be about the same size as a text version, but will typically write out much faster. Of course, when post-processing, you will need to convert it back to text format (see the *binary2txt tool*) or write your own code to read the binary file. The format of the binary file can be understood by looking at the tools/binary2txt.cpp file. This option is only available for the *atom* and *custom* styles.

If the filename ends with ".gz", the dump file (or files, if "*" or "%" is also used) is written in gzipped format. A gzipped dump file will be about 3x smaller than the text version, but will also take longer to write. This option is not available for the *dcd* and *xtc* styles.

Note that in the discussion which follows, for styles which can reference values from a compute or fix, like the *custom*, *cfg*, or *local* styles, the bracketed index I can be specified using a wildcard asterisk with the index to effectively specify multiple values. This takes the form "*" or "*n" or "n*" or "m*n". If N = the size of the vector (for *mode* = scalar) or the number of columns in the array (for *mode* = vector), then an asterisk with no numeric values means all indices from 1 to N. A leading asterisk means all indices from 1 to n (inclusive). A trailing asterisk means all indices from n to N (inclusive). A middle asterisk means all indices from m to n (inclusive).

Using a wildcard is the same as if the individual columns of the array had been listed one by one. E.g. these 2 dump commands are equivalent, since the *compute stress/atom* command creates a per-atom array with 6 columns:

```
compute myPress all stress/atom NULL
dump 2 all custom 100 tmp.dump id myPress[*]
dump 2 all custom 100 tmp.dump id myPress[1] myPress[2] myPress[3] &
                                  myPress[4] myPress[5] myPress[6]
```

This section explains the local attributes that can be specified as part of the *local* style.

The *index* attribute can be used to generate an index number from 1 to N for each line written into the dump file, where N is the total number of local datums from all processors, or lines of output that will appear in the snapshot. Note that because data from different processors depend on what atoms they currently own, and atoms migrate between processor, there is no guarantee that the same index will be used for the same info (e.g. a particular bond) in successive snapshots.

The *c_ID* and *c_ID[I]* attributes allow local vectors or arrays calculated by a *compute* to be output. The ID in the attribute should be replaced by the actual ID of the compute that has been defined previously in the input script. See the *compute* command for details. There are computes for calculating local information such as indices, types, and energies for bonds and angles.

Note that computes which calculate global or per-atom quantities, as opposed to local quantities, cannot be output in a dump local command. Instead, global quantities can be output by the *thermo_style custom* command, and per-atom quantities can be output by the dump custom command.

If *c_ID* is used as a attribute, then the local vector calculated by the compute is printed. If *c_ID[I]* is used, then I must be in the range from 1-M, which will print the Ith column of the local array with M columns calculated by the compute. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

The *f_ID* and *f_ID[I]* attributes allow local vectors or arrays calculated by a *fix* to be output. The ID in the attribute should be replaced by the actual ID of the fix that has been defined previously in the input script.

If *f_ID* is used as a attribute, then the local vector calculated by the fix is printed. If *f_ID[I]* is used, then I must be in the range from 1-M, which will print the Ith column of the local with M columns calculated by the fix. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

Here is an example of how to dump bond info for a system, including the distance and energy of each bond:

```
compute 1 all property/local batom1 batom2 btype
compute 2 all bond/local dist eng
dump 1 all local 1000 tmp.dump index c_1[1] c_1[2] c_1[3] c_2[1] c_2[2]
```

This section explains the atom attributes that can be specified as part of the *custom* and *cfg* styles.

The *id*, *mol*, *proc*, *procp1*, *type*, *element*, *mass*, *vx*, *vy*, *vz*, *fx*, *fy*, *fz*, *q* attributes are self-explanatory.

Id is the atom ID. *Mol* is the molecule ID, included in the data file for molecular systems. *Proc* is the ID of the processor (0 to Nprocs-1) that currently owns the atom. *Procp1* is the proc ID+1, which can be convenient in place of a *type* attribute (1 to Ntypes) for coloring atoms in a visualization program. *Type* is the atom type (1 to Ntypes). *Element* is typically the chemical name of an element, which you must assign to each type via the *dump_modify element* command. More generally, it can be any string you wish to associated with an atom type. *Mass* is the atom mass. *Vx*, *vy*, *vz*, *fx*, *fy*, *fz*, and *q* are components of atom velocity and force and atomic charge.

There are several options for outputting atom coordinates. The *x*, *y*, *z* attributes write atom coordinates "unscaled", in the appropriate distance *units* (Angstroms, sigma, etc). Use *xs*, *ys*, *zs* if you want the coordinates "scaled" to the box size, so that each value is 0.0 to 1.0. If the simulation box is triclinic (tilted), then all atom coords will still be between 0.0 and 1.0. I.e. actual unscaled (x,y,z) = xs*A + ys*B + zs*C, where (A,B,C) are the non-orthogonal vectors of the simulation box edges, as discussed on the *Howto triclinic* doc page.

Use *xu*, *yu*, *zu* if you want the coordinates "unwrapped" by the image flags for each atom. Unwrapped means that if the atom has passed through a periodic boundary one or more times, the value is printed for what the coordinate would be if it had not been wrapped back into the periodic box. Note that using *xu*, *yu*, *zu* means that the coordinate values may be far outside the box bounds printed with the snapshot. Using *xsu*, *ysu*, *zsu* is similar to using *xu*, *yu*, *zu*, except that the unwrapped coordinates are scaled by the box size. Atoms that have passed through a periodic boundary will have the corresponding coordinate increased or decreased by 1.0.

The image flags can be printed directly using the *ix*, *iy*, *iz* attributes. For periodic dimensions, they specify which image of the simulation box the atom is considered to be in. An image of 0 means it is inside the box as defined. A value of 2 means add 2 box lengths to get the true value. A value of -1 means subtract 1 box length to get the true value. LAMMPS updates these flags as atoms cross periodic boundaries during the simulation.

The *mux*, *muy*, *muz* attributes are specific to dipolar systems defined with an atom style of *dipole*. They give the orientation of the atom's point dipole moment. The *mu* attribute gives the magnitude of the atom's dipole moment.

The *radius* and *diameter* attributes are specific to spherical particles that have a finite size, such as those defined with an atom style of *sphere*.

The *omegax*, *omegay*, and *omegaz* attributes are specific to finite-size spherical particles that have an angular velocity. Only certain atom styles, such as *sphere* define this quantity.

The *angmomx*, *angmomy*, and *angmomz* attributes are specific to finite-size aspherical particles that have an angular momentum. Only the *ellipsoid* atom style defines this quantity.

The *tqx*, *tqy*, *tqz* attributes are for finite-size particles that can sustain a rotational torque due to interactions with other particles.

The *c_ID* and *c_ID[I]* attributes allow per-atom vectors or arrays calculated by a *compute* to be output. The ID in the attribute should be replaced by the actual ID of the compute that has been defined previously in the input script. See the *compute* command for details. There are computes for calculating the per-atom energy, stress, centro-symmetry parameter, and coordination number of individual atoms.

Note that computes which calculate global or local quantities, as opposed to per-atom quantities, cannot be output in a dump custom command. Instead, global quantities can be output by the *thermo_style custom* command, and local quantities can be output by the dump local command.

If *c_ID* is used as a attribute, then the per-atom vector calculated by the compute is printed. If *c_ID[I]* is used, then I must be in the range from 1-M, which will print the Ith column of the per-atom array with M columns calculated by the compute. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

The *f_ID* and *f_ID[I]* attributes allow vector or array per-atom quantities calculated by a *fix* to be output. The ID in the attribute should be replaced by the actual ID of the fix that has been defined previously in the input script. The *fix ave/atom* command is one that calculates per-atom quantities. Since it can time-average per-atom quantities produced by any *compute*, *fix*, or atom-style *variable*, this allows those time-averaged results to be written to a dump file.

If *f_ID* is used as a attribute, then the per-atom vector calculated by the fix is printed. If *f_ID[I]* is used, then I must be in the range from 1-M, which will print the Ith column of the per-atom array with M columns calculated by the fix. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

The *v_name* attribute allows per-atom vectors calculated by a *variable* to be output. The name in the attribute should be replaced by the actual name of the variable that has been defined previously in the input script. Only an atom-style variable can be referenced, since it is the only style that generates per-atom values. Variables of style *atom* can reference individual atom attributes, per-atom attributes, thermodynamic keywords, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of creating quantities to output to a dump file.

The *d_name* and *i_name* attributes allow to output custom per atom floating point or integer properties that are managed by *fix property/atom*.

See the *Modify* doc page for information on how to add new compute and fix styles to LAMMPS to calculate per-atom quantities which could then be output into dump files.

15.35.4 Restrictions

To write gzipped dump files, you must either compile LAMMPS with the -DLAMMPS_GZIP option or use the styles from the COMPRESS package. See the *Build settings* doc page for details.

The *atom/gz*, *cfg/gz*, *custom/gz*, and *xyz/gz* styles are part of the COMPRESS package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

The *atom/mpiio*, *cfg/mpiio*, *custom/mpiio*, and *xyz/mpiio* styles are part of the MPIIO package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

The *xtc* style is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

15.35.5 Related commands

dump atom/adios, *dump custom/adios*, *dump h5md*, *dump image*, *dump molfile*, *dump_modify*, *undump*

15.35.6 Default

The defaults for the *image* and *movie* styles are listed on the *dump image* doc page.

15.36 dump atom/adios command

15.37 dump custom/adios command

15.37.1 Syntax

```
dump ID group-ID atom/adios N file.bp

dump ID group-ID custom/adios N file.bp args
```

- ID = user-assigned name for the dump

- group-ID = ID of the group of atoms to be imaged
- adios = style of dump command (other styles *atom* or *cfg* or *dcd* or *xtc* or *xyz* or *local* or *custom* are discussed on the *dump* doc page)
- N = dump every this many timesteps
- file.bp = name of file/stream to write to
- args = same options as in **dump custom** command

15.37.2 Examples

```
dump adios1 all atom/adios   100 atoms.bp
dump 4a     all custom/adios 100 dump_adios.bp id v_p x y z
dump 2 subgroup custom/adios 100 dump_adios.bp mass type xs ys zs vx vy vz
```

15.37.3 Description

Dump a snapshot of atom coordinates every N timesteps in the ADIOS based "BP" file format, or using different I/O solutions in ADIOS, to a stream that can be read on-line by another program. ADIOS-BP files are binary, portable and self-describing.

Use from write_dump:

It is possible to use these dump styles with the *write_dump* command. In this case, the sub-intervals must not be set at all. The write_dump command can be used to create a new file at each individual dump.

```
dump 4     all atom/adios 100 dump.bp
write_dump all atom/adios singledump.bp
```

15.37.4 Restrictions

The number of atoms per snapshot CAN change with the adios style. When using the ADIOS tool 'bpls' to list the content of a .bp file, bpls will print __ for the size of the output table indicating that its size is changing every step.

The *atom/adios* and *custom/adios* dump styles are part of the USER-ADIOS package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

15.37.5 Related commands

dump, *dump_modify*, *undump*

15.38 dump cfg/uef command

15.38.1 Syntax

```
dump ID group-ID cfg/uef N file mass type xs ys zs args
```

- ID = user-assigned name for the dump
- group-ID = ID of the group of atoms to be dumped
- N = dump every this many timesteps
- file = name of file to write dump info to

  `args = same as args for dump custom`

15.38.2 Examples

```
dump 1 all cfg/uef 10 dump.*.cfg mass type xs ys zs
dump 2 all cfg/uef 100 dump.*.cfg mass type xs ys zs id c_stress
```

15.38.3 Description

This command is used to dump atomic coordinates in the reference frame of the applied flow field when *fix nvt/uef* or *fix npt/uef* or is used. Only the atomic coordinates and frame-invariant scalar quantities will be in the flow frame. If velocities are selected as output, for example, they will not be in the same reference frame as the atomic positions.

15.38.4 Restrictions

This fix is part of the USER-UEF package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This command can only be used when *fix nvt/uef* or *fix npt/uef* is active.

15.38.5 Related commands

dump, *fix nvt/uef*

Default: none

15.39 dump h5md command

15.39.1 Syntax

```
dump ID group-ID h5md N file.h5 args
```

- ID = user-assigned name for the dump
- group-ID = ID of the group of atoms to be imaged

- h5md = style of dump command (other styles *atom* or *cfg* or *dcd* or *xtc* or *xyz* or *local* or *custom* are discussed on the *dump* doc page)
- N = dump every this many timesteps
- file.h5 = name of file to write to

```
args = list of data elements to dump, with their dump "sub-intervals"
  position options
  image
  velocity options
  force options
  species options
  file_from ID: do not open a new file, re-use the already opened file from␣
↪dump ID
  box value = yes or no
  create_group value = yes or no
  author value = quoted string
```

Note that at least one element must be specified and image may only be present if position is specified first.

For the elements *position*, *velocity*, *force* and *species*, a sub-interval may be specified to write the data only every N_element iterations of the dump (i.e. every N*N_element time steps). This is specified by this option directly following the element declaration:

```
every N_element
```

15.39.2 Examples

```
dump h5md1 all h5md 100 dump_h5md.h5 position image
dump h5md1 all h5md 100 dump_h5md.h5 position velocity every 10
dump h5md1 all h5md 100 dump_h5md.h5 velocity author "John Doe"
```

15.39.3 Description

Dump a snapshot of atom coordinates every N timesteps in the HDF5 based H5MD file format *(de Buyl)*. HDF5 files are binary, portable and self-describing. This dump style will write only one file, on the root node.

Several dumps may write to the same file, by using file_from and referring to a previously defined dump. Several groups may also be stored within the same file by defining several dumps. A dump that refers (via *file_from*) to an already open dump ID and that concerns another particle group must specify *create_group yes*.

Each data element is written every N*N_element steps. For *image*, no sub-interval is needed as it must be present at the same interval as *position*. *image* must be given after *position* in any case. The box information (edges in each dimension) is stored at the same interval than the *position* element, if present. Else it is stored every N steps.

Note: Because periodic boundary conditions are enforced only on timesteps when neighbor lists are rebuilt, the coordinates of an atom written to a dump file may be slightly outside the simulation box.

Use from write_dump:

It is possible to use this dump style with the *write_dump* command. In this case, the sub-intervals must not be set at all. The write_dump command can be used either to create a new file or to add current data to an existing dump file by using the *file_from* keyword.

Typically, the *species* data is fixed. The following two commands store the position data every 100 timesteps, with the image data, and store once the species data in the same file.

```
dump h5md1 all h5md 100 dump.h5 position image
write_dump all h5md dump.h5 file_from h5md1 species
```

15.39.4 Restrictions

The number of atoms per snapshot cannot change with the h5md style. The position data is stored wrapped (box boundaries not enforced, see note above). Only orthogonal domains are currently supported. This is a limitation of the present dump h5md command and not of H5MD itself.

The *h5md* dump style is part of the USER-H5MD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info. It also requires (i) building the ch5md library provided with LAMMPS (See the *Build package* doc page for more info.) and (ii) having the HDF5 library installed (C bindings are sufficient) on your system. The library ch5md is compiled with the h5cc wrapper provided by the HDF5 library.

15.39.5 Related commands

dump, *dump_modify*, *undump*

(de Buyl) de Buyl, Colberg and Hofling, H5MD: A structured, efficient, and portable file format for molecular data, Comp. Phys. Comm. 185(6), 1546-1553 (2014) - [arXiv:1308.6382].

15.40 dump image command

15.41 dump movie command

15.41.1 Syntax

```
dump ID group-ID style N file color diameter keyword value ...
```

- ID = user-assigned name for the dump
- group-ID = ID of the group of atoms to be imaged
- style = *image* or *movie* = style of dump command (other styles *atom* or *cfg* or *dcd* or *xtc* or *xyz* or *local* or *custom* are discussed on the *dump* doc page)
- N = dump every this many timesteps
- file = name of file to write image to
- color = atom attribute that determines color of each atom
- diameter = atom attribute that determines size of each atom
- zero or more keyword/value pairs may be appended

- keyword = *atom* or *adiam* or *bond* or *line* or *tri* or *body* or *fix* or *size* or *view* or *center* or *up* or *zoom* or *persp* or *box* or *axes* or *subbox* or *shiny* or *ssao*

```
atom = yes/no = do or do not draw atoms
adiam size = numeric value for atom diameter (distance units)
bond values = color width = color and width of bonds
  color = atom or type or none
  width = number or atom or type or none
    number = numeric value for bond width (distance units)
line = color width
  color = type
  width = numeric value for line width (distance units)
tri = color tflag width
  color = type
  tflag = 1 for just triangle, 2 for just tri edges, 3 for both
  width = numeric value for tringle edge width (distance units)
body = color bflag1 bflag2
  color = type
  bflag1,bflag2 = 2 numeric flags to affect how bodies are drawn
fix = fixID color fflag1 fflag2
  fixID = ID of fix that generates objects to dray
  color = type
  fflag1,fflag2 = 2 numeric flags to affect how fix objects are drawn
size values = width height = size of images
  width = width of image in # of pixels
  height = height of image in # of pixels
view values = theta phi = view of simulation box
  theta = view angle from +z axis (degrees)
  phi = azimuthal view angle (degrees)
  theta or phi can be a variable (see below)
center values = flag Cx Cy Cz = center point of image
  flag = "s" for static, "d" for dynamic
  Cx,Cy,Cz = center point of image as fraction of box dimension (0.5 =␣
↪center of box)
  Cx,Cy,Cz can be variables (see below)
up values = Ux Uy Uz = direction that is "up" in image
  Ux,Uy,Uz = components of up vector
  Ux,Uy,Uz can be variables (see below)
zoom value = zfactor = size that simulation box appears in image
  zfactor = scale image size by factor > 1 to enlarge, factor < 1 to␣
↪shrink
  zfactor can be a variable (see below)
persp value = pfactor = amount of "perspective" in image
  pfactor = amount of perspective (0 = none, < 1 = some, > 1 = highly␣
↪skewed)
  pfactor can be a variable (see below)
box values = yes/no diam = draw outline of simulation box
  yes/no = do or do not draw simulation box lines
  diam = diameter of box lines as fraction of shortest box length
axes values = yes/no length diam = draw xyz axes
  yes/no = do or do not draw xyz axes lines next to simulation box
  length = length of axes lines as fraction of respective box lengths
  diam = diameter of axes lines as fraction of shortest box length
subbox values = yes/no diam = draw outline of processor sub-domains
```

```
    yes/no = do or do not draw sub-domain lines
    diam = diameter of sub-domain lines as fraction of shortest box length
  shiny value = sfactor = shinyness of spheres and cylinders
    sfactor = shinyness of spheres and cylinders from 0.0 to 1.0
  ssao value = yes/no seed dfactor = SSAO depth shading
    yes/no = turn depth shading on/off
    seed = random # seed (positive integer)
    dfactor = strength of shading from 0.0 to 1.0
```

15.41.2 Examples

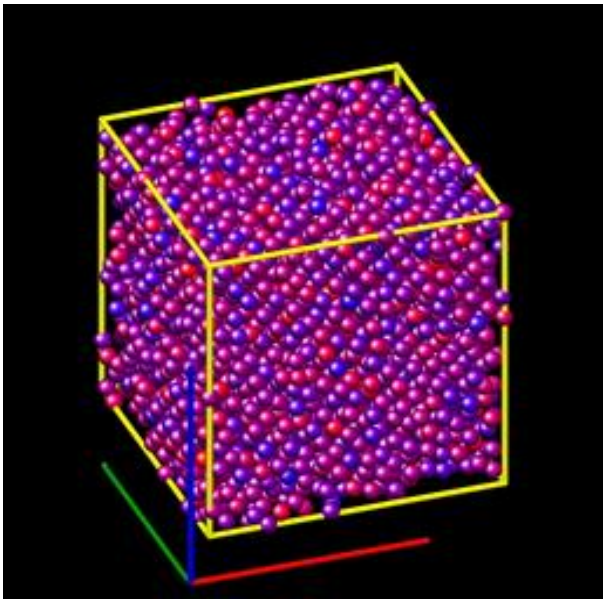
```
dump d0 all image 100 dump.\*.jpg type type
dump d1 mobile image 500 snap.\*.png element element ssao yes 4539 0.6
dump d2 all image 200 img-\*.ppm type type zoom 2.5 adiam 1.5 size 1280 720
dump m0 all movie 1000 movie.mpg type type size 640 480
dump m1 all movie 1000 movie.avi type type size 640 480
dump m2 all movie 100 movie.m4v type type zoom 1.8 adiam v_value size 1280 720
```

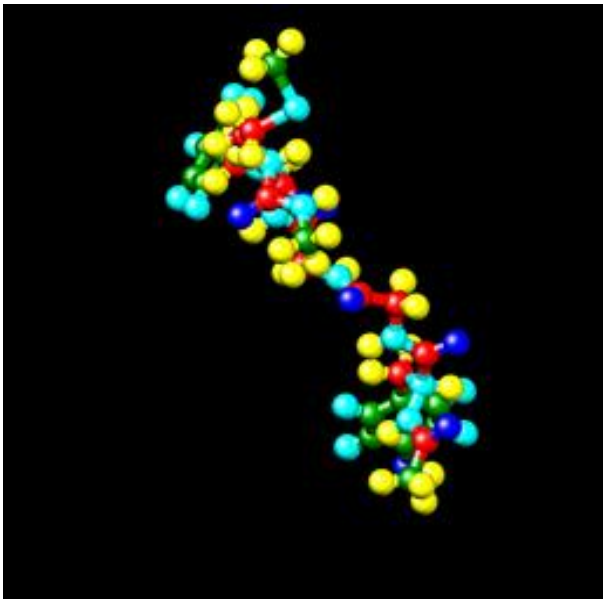
15.41.3 Description

Dump a high-quality rendered image of the atom configuration every N timesteps and save the images either as a sequence of JPEG or PNG or PPM files, or as a single movie file. The options for this command as well as the *dump_modify* command control what is included in the image or movie and how it appears. A series of such images can easily be manually converted into an animated movie of your simulation or the process can be automated without writing the intermediate files using the dump movie style; see further details below. Other dump styles store snapshots of numerical data associated with atoms in various formats, as discussed on the *dump* doc page.

Note that a set of images or a movie can be made after a simulation has been run, using the *rerun* command to read snapshots from an existing dump file, and using these dump commands in the rerun script to generate the images/movie.

Here are two sample images, rendered as 1024x1024 JPEG files. Click to see the full-size images:





Only atoms in the specified group are rendered in the image. The *dump_modify region and thresh* commands can also alter what atoms are included in the image. The filename suffix determines whether a JPEG, PNG, or PPM file is created with the *image* dump style. If the suffix is ".jpg" or ".jpeg", then a JPEG format file is created, if the suffix is ".png", then a PNG format is created, else a PPM (aka NETPBM) format file is created. The JPEG and PNG files are binary; PPM has a text mode header followed by binary data. JPEG images have lossy compression; PNG has lossless compression; and PPM files are uncompressed but can be compressed with gzip, if LAMMPS has been compiled with -DLAMMPS_GZIP and a ".gz" suffix is used.

Similarly, the format of the resulting movie is chosen with the *movie* dump style. This is handled by the underlying FFmpeg converter and thus details have to be looked up in the FFmpeg documentation. Typical examples are: .avi, .mpg, .m4v, .mp4, .mkv, .flv, .mov, .gif Additional settings of the movie compression like bitrate and framerate can be set using the *dump_modify* command.

To write out JPEG and PNG format files, you must build LAMMPS with support for the corresponding JPEG or PNG library. To convert images into movies, LAMMPS has to be compiled with the -DLAMMPS_FFMPEG flag. See the *Build settings* doc page for details.

Note: Because periodic boundary conditions are enforced only on timesteps when neighbor lists are rebuilt, the coordinates of an atom in the image may be slightly outside the simulation box.

Dumps are performed on timesteps that are a multiple of N (including timestep 0) and on the last timestep of a minimization if the minimization converges. Note that this means a dump will not be performed on the initial timestep after the dump command is invoked, if the current timestep is not a multiple of N. This behavior can be changed via the *dump_modify first* command, which can be useful if the dump command is invoked after a minimization ended on an arbitrary timestep. N can be changed between runs by using the *dump_modify every* command.

Dump *image* filenames must contain a wildcard character "*", so that one image file per snapshot is written. The "*" character is replaced with the timestep value. For example, tmp.dump.*.jpg becomes tmp.dump.0.jpg, tmp.dump.10000.jpg, tmp.dump.20000.jpg, etc. Note that the *dump_modify pad* command can be used to insure all timestep numbers are the same length (e.g. 00010), which can make it easier to convert a series of images into a movie in the correct ordering.

Dump *movie* filenames on the other hand, must not have any wildcard character since only one file combining all images into a single movie will be written by the movie encoder.

The *color* and *diameter* settings determine the color and size of atoms rendered in the image. They can be any atom attribute defined for the *dump custom* command, including *type* and *element*. This includes per-atom quantities calculated by a *compute*, *fix*, or *variable*, which are prefixed by "c_", "f_", or "v_" respectively. Note that the *diameter* setting can be overridden with a numeric value applied to all atoms by the optional *adiam* keyword.

If *type* is specified for the *color* setting, then the color of each atom is determined by its atom type. By default the mapping of types to colors is as follows:

- type 1 = red
- type 2 = green
- type 3 = blue
- type 4 = yellow
- type 5 = aqua
- type 6 = cyan

and repeats itself for types > 6. This mapping can be changed by the *dump_modify acolor* command.

If *type* is specified for the *diameter* setting then the diameter of each atom is determined by its atom type. By default all types have diameter 1.0. This mapping can be changed by the *dump_modify adiam* command.

If *element* is specified for the *color* and/or *diameter* setting, then the color and/or diameter of each atom is determined by which element it is, which in turn is specified by the element-to-type mapping specified by the "dump_modify element" command. By default every atom type is C (carbon). Every element has a color and diameter associated with it, which is the same as the colors and sizes used by the AtomEye visualization package.

If other atom attributes are used for the *color* or *diameter* settings, they are interpreted in the following way.

If "vx", for example, is used as the *color* setting, then the color of the atom will depend on the x-component of its velocity. The association of a per-atom value with a specific color is determined by a "color map", which can be specified via the *dump_modify* command. The basic idea is that the atom-attribute will be within a range of values, and every value within the range is mapped to a specific color. Depending on how the color map is defined, that mapping can take place via interpolation so that a value of -3.2 is halfway between "red" and "blue", or discretely so that the value of -3.2 is "orange".

If "vx", for example, is used as the *diameter* setting, then the atom will be rendered using the x-component of its velocity as the diameter. If the per-atom value <= 0.0, them the atom will not be drawn. Note that finite-size spherical particles, as defined by *atom_style sphere* define a per-particle radius or diameter, which can be used as the *diameter* setting.

The various keywords listed above control how the image is rendered. As listed below, all of the keywords have defaults, most of which you will likely not need to change. The *dump modify* also has options specific to the dump image style, particularly for assigning colors to atoms, bonds, and other image features.

The *atom* keyword allow you to turn off the drawing of all atoms, if the specified value is *no*. Note that this will not turn off the drawing of particles that are represented as lines, triangles, or bodies, as discussed below. These particles can be drawn separately if the *line*, *tri*, or *body* keywords are used.

The *adiam* keyword allows you to override the *diameter* setting to set a single numeric *size*. All atoms will be drawn with that diameter, e.g. 1.5, which is in whatever distance *units* the input script defines, e.g. Angstroms.

The *bond* keyword allows to you to alter how bonds are drawn. A bond is only drawn if both atoms in the bond are being drawn due to being in the specified group and due to other selection criteria (e.g. region, threshold settings of the *dump_modify* command). By default, bonds are drawn if they are defined in the input data file as read by the *read_data* command. Using *none* for both the bond *color* and *width* value will turn off the drawing of all bonds.

If *atom* is specified for the bond *color* value, then each bond is drawn in 2 halves, with the color of each half being the color of the atom at that end of the bond.

If *type* is specified for the *color* value, then the color of each bond is determined by its bond type. By default the mapping of bond types to colors is as follows:

- type 1 = red
- type 2 = green
- type 3 = blue
- type 4 = yellow
- type 5 = aqua
- type 6 = cyan

and repeats itself for bond types > 6. This mapping can be changed by the *dump_modify bcolor* command.

The bond *width* value can be a numeric value or *atom* or *type* (or *none* as indicated above).

If a numeric value is specified, then all bonds will be drawn as cylinders with that diameter, e.g. 1.0, which is in whatever distance *units* the input script defines, e.g. Angstroms.

If *atom* is specified for the *width* value, then each bond will be drawn with a width corresponding to the minimum diameter of the 2 atoms in the bond.

If *type* is specified for the *width* value then the diameter of each bond is determined by its bond type. By default all types have diameter 0.5. This mapping can be changed by the *dump_modify bdiam* command.

The *line* keyword can be used when *atom_style line* is used to define particles as line segments, and will draw them as lines. If this keyword is not used, such particles will be drawn as spheres, the same as if they were regular atoms. The only setting currently allowed for the *color* value is *type*, which will color the lines according to the atom type of the particle. By default the mapping of types to colors is as follows:

- type 1 = red
- type 2 = green
- type 3 = blue
- type 4 = yellow
- type 5 = aqua
- type 6 = cyan

and repeats itself for types > 6. There is not yet an option to change this via the *dump_modify* command.

The line *width* can only be a numeric value, which specifies that all lines will be drawn as cylinders with that diameter, e.g. 1.0, which is in whatever distance *units* the input script defines, e.g. Angstroms.

The *tri* keyword can be used when *atom_style tri* is used to define particles as triangles, and will draw them as triangles or edges (3 lines) or both, depending on the setting for *tflag*. If edges are drawn, the *width* setting determines the diameters of the line segments. If this keyword is not used, triangle particles will be drawn as spheres, the same as if they were regular atoms. The only setting currently allowed for the *color* value is *type*, which will color the triangles according to the atom type of the particle. By default the mapping of types to colors is as follows:

- type 1 = red
- type 2 = green
- type 3 = blue
- type 4 = yellow
- type 5 = aqua
- type 6 = cyan

and repeats itself for types > 6. There is not yet an option to change this via the *dump_modify* command.

The *body* keyword can be used when *atom_style body* is used to define body particles with internal state (e.g. sub-particles), and will drawn them in a manner specific to the body style. If this keyword is not used, such particles will be drawn as spheres, the same as if they were regular atoms.

The *Howto body* doc page describes the body styles LAMMPS currently supports, and provides more details as to the kind of body particles they represent and how they are drawn by this dump image command. For all the body styles, individual atoms can be either a body particle or a usual point (non-body) particle. Non-body particles will be drawn the same way they would be as a regular atom. The *bflag1* and *bflag2* settings are numerical values which are passed to the body style to affect how the drawing of a body particle is done. See the *Howto body* doc page for a description of what these parameters mean for each body style.

The only setting currently allowed for the *color* value is *type*, which will color the body particles according to the atom type of the particle. By default the mapping of types to colors is as follows:

- type 1 = red
- type 2 = green
- type 3 = blue
- type 4 = yellow
- type 5 = aqua
- type 6 = cyan

and repeats itself for types > 6. There is not yet an option to change this via the *dump_modify* command.

The *fix* keyword can be used with a *fix* that produces objects to be drawn.

The *fflag1* and *fflag2* settings are numerical values which are passed to the fix to affect how the drawing of its objects is done. See the individual fix doc page for a description of what these parameters mean for a particular fix.

The only setting currently allowed for the *color* value is *type*, which will color the fix objects according to their type. By default the mapping of types to colors is as follows:

- type 1 = red
- type 2 = green
- type 3 = blue
- type 4 = yellow
- type 5 = aqua
- type 6 = cyan

and repeats itself for types > 6. There is not yet an option to change this via the *dump_modify* command.

The *size* keyword sets the width and height of the created images, i.e. the number of pixels in each direction.

The *view*, *center*, *up*, *zoom*, and *persp* values determine how 3d simulation space is mapped to the 2d plane of the image. Basically they control how the simulation box appears in the image.

All of the *view*, *center*, *up*, *zoom*, and *persp* values can be specified as numeric quantities, whose meaning is explained below. Any of them can also be specified as an *equal-style variable*, by using v_name as the value, where "name" is the variable name. In this case the variable will be evaluated on the timestep each image is created to create a new value. If the equal-style variable is time-dependent, this is a means of changing the way the simulation box appears from image to image, effectively doing a pan or fly-by view of your simulation.

The *view* keyword determines the viewpoint from which the simulation box is viewed, looking towards the *center* point. The *theta* value is the vertical angle from the +z axis, and must be an angle from 0 to 180 degrees. The *phi* value is an azimuthal angle around the z axis and can be positive or negative. A value of 0.0 is a view along the +x axis, towards the *center* point. If *theta* or *phi* are specified via variables, then the variable values should be in degrees.

The *center* keyword determines the point in simulation space that will be at the center of the image. *Cx*, *Cy*, and *Cz* are specified as fractions of the box dimensions, so that (0.5,0.5,0.5) is the center of the simulation box. These values do not have to be between 0.0 and 1.0, if you want the simulation box to be offset from the center of the image. Note, however, that if you choose strange values for *Cx*, *Cy*, or *Cz* you may get a blank image. Internally, *Cx*, *Cy*, and *Cz* are converted into a point in simulation space. If *flag* is set to "s" for static, then this conversion is done once, at the time the dump command is issued. If *flag* is set to "d" for dynamic then the conversion is performed every time a new image is created. If the box size or shape is changing, this will adjust the center point in simulation space.

The *up* keyword determines what direction in simulation space will be "up" in the image. Internally it is stored as a vector that is in the plane perpendicular to the view vector implied by the *theta* and *pni* values, and which is also in the plane defined by the view vector and user-specified up vector. Thus this internal vector is computed from the user-specified *up* vector as

```
up_internal = view cross (up cross view)
```

This means the only restriction on the specified *up* vector is that it cannot be parallel to the *view* vector, implied by the *theta* and *phi* values.

The *zoom* keyword scales the size of the simulation box as it appears in the image. The default *zfactor* value of 1 should display an image mostly filled by the atoms in the simulation box. A *zfactor* > 1 will make the simulation box larger; a *zfactor* < 1 will make it smaller. *Zfactor* must be a value > 0.0.

The *persp* keyword determines how much depth perspective is present in the image. Depth perspective makes lines that are parallel in simulation space appear non-parallel in the image. A *pfactor* value of 0.0 means that parallel lines will meet at infinity (1.0/pfactor), which is an orthographic rendering with no perspective. A *pfactor* value between 0.0 and 1.0 will introduce more perspective. A *pfactor* value > 1 will create a highly skewed image with a large amount of perspective.

Note: The *persp* keyword is not yet supported as an option.

The *box* keyword determines if and how the simulation box boundaries are rendered as thin cylinders in the image. If *no* is set, then the box boundaries are not drawn and the *diam* setting is ignored. If *yes* is set, the 12 edges of the box are drawn, with a diameter that is a fraction of the shortest box length in x,y,z (for 3d) or x,y (for 2d). The color of the box boundaries can be set with the *dump_modify boxcolor* command.

The *axes* keyword determines if and how the coordinate axes are rendered as thin cylinders in the image. If *no* is set, then the axes are not drawn and the *length* and *diam* settings are ignored. If *yes* is set, 3 thin cylinders are drawn to represent the x,y,z axes in colors red,green,blue. The origin of these cylinders will be offset from the lower left corner of the box by 10%. The *length* setting determines how long the cylinders will be as a fraction of the respective box lengths. The *diam* setting determines their thickness as a fraction of the shortest box length in x,y,z (for 3d) or x,y (for 2d).

The *subbox* keyword determines if and how processor sub-domain boundaries are rendered as thin cylinders in the image. If *no* is set (default), then the sub-domain boundaries are not drawn and the *diam* setting is ignored. If *yes* is set, the 12 edges of each processor sub-domain are drawn, with a diameter that is a fraction of the shortest box length in x,y,z (for 3d) or x,y (for 2d). The color of the sub-domain boundaries can be set with the *dump_modify boxcolor* command.

The *shiny* keyword determines how shiny the objects rendered in the image will appear. The *sfactor* value must be a value 0.0 <= *sfactor* <= 1.0, where *sfactor* = 1 is a highly reflective surface and *sfactor* = 0 is a rough non-shiny surface.

The *ssao* keyword turns on/off a screen space ambient occlusion (SSAO) model for depth shading. If *yes* is set, then atoms further away from the viewer are darkened via a randomized process, which is perceived as depth. The calculation of this effect can increase the cost of computing the image by roughly 2x. The strength of the effect can be scaled by the *dfactor* parameter. If *no* is set, no depth shading is performed.

A series of JPEG, PNG, or PPM images can be converted into a movie file and then played as a movie using commonly available tools. Using dump style *movie* automates this step and avoids the intermediate step of writing (many) image snapshot file. But LAMMPS has to be compiled with -DLAMMPS_FFMPEG and an FFmpeg executable have to be installed.

To manually convert JPEG, PNG or PPM files into an animated GIF or MPEG or other movie file you can use:

- a) Use the ImageMagick convert program.

```
% convert *.jpg foo.gif
% convert -loop 1 *.ppm foo.mpg
```

  Animated GIF files from ImageMagick are not optimized. You can use a program like gifsicle to optimize and thus massively shrink them. MPEG files created by ImageMagick are in MPEG-1 format with a rather inefficient compression and low quality compared to more modern compression styles like MPEG-4, H.264, VP8, VP9, H.265 and so on.

- b) Use QuickTime.

  Select "Open Image Sequence" under the File menu Load the images into QuickTime to animate them Select "Export" under the File menu Save the movie as a QuickTime movie (*.mov) or in another format. QuickTime can generate very high quality and efficiently compressed movie files. Some of the supported formats require to buy a license and some are not readable on all platforms until specific runtime libraries are installed.

- c) Use FFmpeg

  FFmpeg is a command line tool that is available on many platforms and allows extremely flexible encoding and decoding of movies.

```
cat snap.*.jpg | ffmpeg -y -f image2pipe -c:v mjpeg -i - -b:v 2000k movie.m4v
cat snap.*.ppm | ffmpeg -y -f image2pipe -c:v ppm -i - -b:v 2400k movie.avi
```

  Front ends for FFmpeg exist for multiple platforms. For more information see the FFmpeg homepage

---

Play the movie:

- a) Use your browser to view an animated GIF movie.

  Select "Open File" under the File menu Load the animated GIF file

- b) Use the freely available mplayer or ffplay tool to view a movie. Both are available for multiple OSes and support a large variety of file formats and decoders.

```
% mplayer foo.mpg
% ffplay bar.avi
```

- c) Use the Pizza.py animate tool, which works directly on a series of image files.

```
a = animate("foo*.jpg")
```

- d) QuickTime and other Windows- or MacOS-based media players can obviously play movie files directly. Similarly for corresponding tools bundled with Linux desktop environments. However, due to licensing issues with some file formats, the formats may require installing additional libraries, purchasing a license, or may not be supported.

See the *Modify* doc page for information on how to add new compute and fix styles to LAMMPS to calculate per-atom quantities which could then be output into dump files.

15.41.4 Restrictions

To write JPEG images, you must use the -DLAMMPS_JPEG switch when building LAMMPS and link with a JPEG library. To write PNG images, you must use the -DLAMMPS_PNG switch when building LAMMPS and link with a PNG library.

To write *movie* dumps, you must use the -DLAMMPS_FFMPEG switch when building LAMMPS and have the FFmpeg executable available on the machine where LAMMPS is being run. Typically it's name is lowercase, i.e. ffmpeg.

See the *Build settings* doc page for details.

Note that since FFmpeg is run as an external program via a pipe, LAMMPS has limited control over its execution and no knowledge about errors and warnings printed by it. Those warnings and error messages will be printed to the screen only. Due to the way image data is communicated to FFmpeg, it will often print the message

```
pipe:: Input/output error
```

which can be safely ignored. Other warnings and errors have to be addressed according to the FFmpeg documentation. One known issue is that certain movie file formats (e.g. MPEG level 1 and 2 format streams) have video bandwidth limits that can be crossed when rendering too large of image sizes. Typical warnings look like this:

```
[mpeg @ 0x98b5e0] packet too large, ignoring buffer limits to mux it
[mpeg @ 0x98b5e0] buffer underflow st=0 bufi=281407 size=285018
[mpeg @ 0x98b5e0] buffer underflow st=0 bufi=283448 size=285018
```

In this case it is recommended to either reduce the size of the image or encode in a different format that is also supported by your copy of FFmpeg, and which does not have this limitation (e.g. .avi, .mkv, mp4).

15.41.5 Related commands

dump, *dump_modify*, *undump*

15.41.6 Default

The defaults for the keywords are as follows:

- adiam = not specified (use diameter setting)
- atom = yes
- bond = none none (if no bonds in system)
- bond = atom 0.5 (if bonds in system)
- size = 512 512
- view = 60 30 (for 3d)
- view = 0 0 (for 2d)
- center = s 0.5 0.5 0.5
- up = 0 0 1 (for 3d)
- up = 0 1 0 (for 2d)
- zoom = 1.0
- persp = 0.0
- box = yes 0.02
- axes = no 0.0 0.0
- subbox no 0.0
- shiny = 1.0
- ssao = no

15.42 dump_modify command

15.42.1 Syntax

```
dump_modify dump-ID keyword values ...
```

- dump-ID = ID of dump to modify
- one or more keyword/value pairs may be appended
- these keywords apply to various dump styles
- keyword = *append* or *at* or *buffer* or *delay* or *element* or *every* or *fileper* or *first* or *flush* or *format* or *image* or *label* or *maxfiles* or *nfile* or *pad* or *pbc* or *precision* or *region* or *refresh* or *scale* or *sfactor* or *sort* or *tfactor* or *thermo* or *thresh* or *time* or *units* or *unwrap*

```
append arg = yes or no
at arg = N
  N = index of frame written upon first dump
buffer arg = yes or no
delay arg = Dstep
  Dstep = delay output until this timestep
element args = E1 E2 ... EN, where N = # of atom types
  E1,...,EN = element name, e.g. C or Fe or Ga
every arg = N
  N = dump every this many timesteps
  N can be a variable (see below)
fileper arg = Np
  Np = write one file for every this many processors
first arg = yes or no
flush arg = yes or no
format args = line string, int string, float string, M string, or none
  string = C-style format string
  M = integer from 1 to N, where N = # of per-atom quantities being output
image arg = yes or no
label arg = string
  string = character string (e.g. BONDS) to use in header of dump local␣
↪file
maxfiles arg = Fmax
  Fmax = keep only the most recent Fmax snapshots (one snapshot per file)
nfile arg = Nf
  Nf = write this many files, one from each of Nf processors
pad arg = Nchar = # of characters to convert timestep to
pbc arg = yes or no = remap atoms via periodic boundary conditions
precision arg = power-of-10 value from 10 to 1000000
region arg = region-ID or "none"
refresh arg = c_ID = compute ID that supports a refresh operation
scale arg = yes or no
sfactor arg = coordinate scaling factor (> 0.0)
sort arg = off or id or N or -N
   off = no sorting of per-atom lines within a snapshot
   id = sort per-atom lines by atom ID
   N = sort per-atom lines in ascending order by the Nth column
   -N = sort per-atom lines in descending order by the Nth column
tfactor arg = time scaling factor (> 0.0)
thermo arg = yes or no
time arg = yes or no
thresh args = attribute operator value
  attribute = same attributes (x,fy,etotal,sxx,etc) used by dump custom␣
↪style
  operator = "<" or "<=" or ">" or ">=" or "==" or "!=" or "|^"
  value = numeric value to compare to, or LAST
  these 3 args can be replaced by the word "none" to turn off thresholding
units arg = yes or no
unwrap arg = yes or no
```

- these keywords apply only to the *image* and *movie* *styles*
- keyword = *acolor* or *adiam* or *amap* or *backcolor* or *bcolor* or *bdiam* or *boxcolor* or *color* or *bitrate* or *framerate*

```
acolor args = type color
```

```
  type = atom type or range of types (see below)
  color = name of color or color1/color2/...
adiam args = type diam
  type = atom type or range of types (see below)
  diam = diameter of atoms of that type (distance units)
amap args = lo hi style delta N entry1 entry2 ... entryN
  lo = number or min = lower bound of range of color map
  hi = number or max = upper bound of range of color map
  style = 2 letters = "c" or "d" or "s" plus "a" or "f"
    "c" for continuous
    "d" for discrete
    "s" for sequential
    "a" for absolute
    "f" for fractional
  delta = binsize (only used for style "s", otherwise ignored)
    binsize = range is divided into bins of this width
  N = # of subsequent entries
  entry = value color (for continuous style)
    value = number or min or max = single value within range
    color = name of color used for that value
  entry = lo hi color (for discrete style)
    lo/hi = number or min or max = lower/upper bound of subset of range
    color = name of color used for that subset of values
  entry = color (for sequential style)
    color = name of color used for a bin of values
backcolor arg = color
  color = name of color for background
bcolor args = type color
  type = bond type or range of types (see below)
  color = name of color or color1/color2/...
bdiam args = type diam
  type = bond type or range of types (see below)
  diam = diameter of bonds of that type (distance units)
boxcolor arg = color
  color = name of color for simulation box lines and processor sub-domain␣
↪lines
color args = name R G B
  name = name of color
  R,G,B = red/green/blue numeric values from 0.0 to 1.0
bitrate arg = rate
  rate = target bitrate for movie in kbps
framerate arg = fps
  fps = frames per second for movie
```

15.42.2 Examples

```
dump_modify 1 format line "%d %d %20.15g %g %g" scale yes
dump_modify 1 format float %20.15g scale yes
dump_modify myDump image yes scale no flush yes
dump_modify 1 region mySphere thresh x < 0.0 thresh epair >= 3.2
dump_modify xtcdump precision 10000 sfactor 0.1
dump_modify 1 every 1000 nfile 20
dump_modify 1 every v_myVar
dump_modify 1 amap min max cf 0.0 3 min green 0.5 yellow max blue boxcolor red
```

15.42.3 Description

Modify the parameters of a previously defined dump command. Not all parameters are relevant to all dump styles.

As explained on the *dump* doc page, the *atom/mpiio*, *custom/mpiio*, and *xyz/mpiio* dump styles are identical in command syntax and in the format of the dump files they create, to the corresponding styles without "mpiio", except the single dump file they produce is written in parallel via the MPI-IO library. Thus if a dump_modify option below is valid for the *atom* style, it is also valid for the *atom/mpiio* style, and similarly for the other styles which allow for use of MPI-IO.

These keywords apply to various dump styles, including the *dump image* and *dump movie* styles. The description gives details.

The *append* keyword applies to all dump styles except *cfg* and *xtc* and *dcd*. It also applies only to text output files, not to binary or gzipped or image/movie files. If specified as *yes*, then dump snapshots are appended to the end of an existing dump file. If specified as *no*, then a new dump file will be created which will overwrite an existing file with the same name.

The *at* keyword only applies to the *netcdf* dump style. It can only be used if the *append yes* keyword is also used. The *N* argument is the index of which frame to append to. A negative value can be specified for *N*, which means a frame counted from the end of the file. The *at* keyword can only be used if the dump_modify command is before the first command that causes dump snapshots to be output, e.g. a *run* or *minimize* command. Once the dump file has been opened, this keyword has no further effect.

The *buffer* keyword applies only to dump styles *atom*, *cfg*, *custom*, *local*, and *xyz*. It also applies only to text output files, not to binary or gzipped files. If specified as *yes*, which is the default, then each processor writes its output into an internal text buffer, which is then sent to the processor(s) which perform file writes, and written by those processors(s) as one large chunk of text. If specified as *no*, each processor sends its per-atom data in binary format to the processor(s) which perform file wirtes, and those processor(s) format and write it line by line into the output file.

The buffering mode is typically faster since each processor does the relatively expensive task of formatting the output for its own atoms. However it requires about twice the memory (per processor) for the extra buffering.

The *delay* keyword applies to all dump styles. No snapshots will be output until the specified *Dstep* timestep or later. Specifying *Dstep* < 0 is the same as turning off the delay setting. This is a way to turn off unwanted output early in a simulation, for example, during an equilibration phase.

The *element* keyword applies only to the dump *cfg*, *xyz*, and *image* styles. It associates element names (e.g. H, C, Fe) with LAMMPS atom types. See the list of element names at the bottom of this page.

In the case of dump *cfg*, this allows the AtomEye visualization package to read the dump file and render atoms with the appropriate size and color.

In the case of dump *image*, the output images will follow the same AtomEye convention. An element name is specified for each atom type (1 to Ntype) in the simulation. The same element name can be given to multiple atom types.

In the case of *xyz* format dumps, there are no restrictions to what label can be used as an element name. Any white-space separated text will be accepted.

The *every* keyword changes the dump frequency originally specified by the *dump* command to a new value. The every keyword can be specified in one of two ways. It can be a numeric value in which case it must be > 0. Or it can be an *equal-style variable*, which should be specified as v_name, where name is the variable name.

In this case, the variable is evaluated at the beginning of a run to determine the next timestep at which a dump snapshot will be written out. On that timestep the variable will be evaluated again to determine the next timestep, etc. Thus the variable should return timestep values. See the stagger() and logfreq() and stride() math functions for *equal-style variables*, as examples of useful functions to use in this context. Other similar math functions could easily be added as options for *equal-style variables*. Also see the next() function, which allows use of a file-style variable which reads successive values from a file, each time the variable is evaluated. Used with the *every* keyword, if the file contains a list of ascending timesteps, you can output snapshots whenever you wish.

Note that when using the variable option with the *every* keyword, you need to use the *first* option if you want an initial snapshot written to the dump file. The *every* keyword cannot be used with the dump *dcd* style.

For example, the following commands will write snapshots at timesteps 0,10,20,30,100,200,300,1000,2000,etc:

```
variable        s equal logfreq(10,3,10)
dump            1 all atom 100 tmp.dump
dump_modify     1 every v_s first yes
```

The following commands would write snapshots at the timesteps listed in file tmp.times:

```
variable        f file tmp.times
variable        s equal next(f)
dump            1 all atom 100 tmp.dump
dump_modify     1 every v_s
```

Note: When using a file-style variable with the *every* keyword, the file of timesteps must list a first timestep that is beyond the current timestep (e.g. it cannot be 0). And it must list one or more timesteps beyond the length of the run you perform. This is because the dump command will generate an error if the next timestep it reads from the file is not a value greater than the current timestep. Thus if you wanted output on steps 0,15,100 of a 100-timestep run, the file should contain the values 15,100,101 and you should also use the dump_modify first command. Any final value > 100 could be used in place of 101.

The *first* keyword determines whether a dump snapshot is written on the very first timestep after the dump command is invoked. This will always occur if the current timestep is a multiple of N, the frequency specified in the *dump* command, including timestep 0. But if this is not the case, a dump snapshot will only be written if the setting of this keyword is *yes*. If it is *no*, which is the default, then it will not be written.

The *flush* keyword determines whether a flush operation is invoked after a dump snapshot is written to the dump file. A flush insures the output in that file is current (no buffering by the OS), even if LAMMPS halts before the simulation completes. Flushes cannot be performed with dump style *xtc*.

The *format* keyword can be used to change the default numeric format output by the text-based dump styles: *atom*, *custom*, *cfg*, and *xyz* styles, and their MPIIO variants. Only the *line* or *none* options can be used with the *atom* and *xyz* styles.

All the specified format strings are C-style formats, e.g. as used by the C/C++ printf() command. The *line* keyword takes a single argument which is the format string for an entire line of output for each atom (do not include a trailing "n"), with N fields, which you must enclose in quotes if it is more than one field. The *int* and *float* keywords take a single format argument and are applied to all integer or floating-point quantities output. The setting for *M string* also takes a single format argument which is used for the Mth value output in each line, e.g. the 5th column is output in high precision for "format 5 %20.15g".

Note: When using the *line* keyword for the *cfg* style, the first two fields (atom ID and type) are not actually written into the CFG file, however you must include formats for them in the format string.

The *format* keyword can be used multiple times. The precedence is that for each value in a line of output, the *M* format (if specified) is used, else the *int* or *float* setting (if specified) is used, else the *line* setting (if specified) for that value is used, else the default setting is used. A setting of *none* clears all previous settings, reverting all values to their default format.

Note: Atom and molecule IDs are stored internally as 4-byte or 8-byte signed integers, depending on how LAMMPS was compiled. When specifying the *format int* option you can use a "%d"-style format identifier in the format string and LAMMPS will convert this to the corresponding 8-byte form if it is needed when outputting those values. However, when specifying the *line* option or *format M string* option for those values, you should specify a format string appropriate for an 8-byte signed integer, e.g. one with "%ld", if LAMMPS was compiled with the -DLAMMPS_BIGBIG option for 8-byte IDs.

Note: Any value written to a text-based dump file that is a per-atom quantity calculated by a *compute* or *fix* is stored internally as a floating-point value. If the value is actually an integer and you wish it to appear in the text dump file as a (large) integer, then you need to use an appropriate format. For example, these commands:

```
compute     1 all property/local batom1 batom2
dump        1 all local 100 tmp.bonds index c_1[1] c_1[2]
dump_modify 1 format "%d %0.0f %0.0f"
```

will output the two atom IDs for atoms in each bond as integers. If the dump_modify command were omitted, they would appear as floating-point values, assuming they were large integers (more than 6 digits). The "index" keyword should use the "%d" format since it is not generated by a compute or fix, and is stored internally as an integer.

The *fileper* keyword is documented below with the *nfile* keyword.

The *image* keyword applies only to the dump *atom* style. If the image value is *yes*, 3 flags are appended to each atom's coords which are the absolute box image of the atom in each dimension. For example, an x image flag of -2 with a normalized coord of 0.5 means the atom is in the center of the box, but has passed through the box boundary 2 times

and is really 2 box lengths to the left of its current coordinate. Note that for dump style *custom* these various values can be printed in the dump file by using the appropriate atom attributes in the dump command itself.

The *label* keyword applies only to the dump *local* style. When it writes local information, such as bond or angle topology to a dump file, it will use the specified *label* to format the header. By default this includes 2 lines:

```
ITEM: NUMBER OF ENTRIES
ITEM: ENTRIES ...
```

The word "ENTRIES" will be replaced with the string specified, e.g. BONDS or ANGLES.

The *maxfiles* keyword can only be used when a '*' wildcard is included in the dump file name, i.e. when writing a new file(s) for each snapshot. The specified *Fmax* is how many snapshots will be kept. Once this number is reached, the file(s) containing the oldest snapshot is deleted before a new dump file is written. If the specified *Fmax* <= 0, then all files are retained.

This can be useful for debugging, especially if you don't know on what timestep something bad will happen, e.g. when LAMMPS will exit with an error. You can dump every timestep, and limit the number of dump files produced, even if you run for 1000s of steps.

The *nfile* or *fileper* keywords can be used in conjunction with the "%" wildcard character in the specified dump file name, for all dump styles except the *dcd*, *image*, *movie*, *xtc*, and *xyz* styles (for which "%" is not allowed). As explained on the *dump* command doc page, the "%" character causes the dump file to be written in pieces, one piece for each of P processors. By default P = the number of processors the simulation is running on. The *nfile* or *fileper* keyword can be used to set P to a smaller value, which can be more efficient when running on a large number of processors.

The *nfile* keyword sets P to the specified Nf value. For example, if Nf = 4, and the simulation is running on 100 processors, 4 files will be written, by processors 0,25,50,75. Each will collect information from itself and the next 24 processors and write it to a dump file.

For the *fileper* keyword, the specified value of Np means write one file for every Np processors. For example, if Np = 4, every 4th processor (0,4,8,12,etc) will collect information from itself and the next 3 processors and write it to a dump file.

The *pad* keyword only applies when the dump filename is specified with a wildcard "*" character which becomes the timestep. If *pad* is 0, which is the default, the timestep is converted into a string of unpadded length, e.g. 100 or 12000 or 2000000. When *pad* is specified with *Nchar* > 0, the string is padded with leading zeroes so they are all the same length = *Nchar*. For example, pad 7 would yield 0000100, 0012000, 2000000. This can be useful so that post-processing programs can easily read the files in ascending timestep order.

The *pbc* keyword applies to all the dump styles. As explained on the *dump* doc page, atom coordinates in a dump file may be slightly outside the simulation box. This is because periodic boundary conditions are enforced only on timesteps when neighbor lists are rebuilt, which will not typically coincide with the timesteps dump snapshots are written. If the setting of this keyword is set to *yes*, then all atoms will be remapped to the periodic box before the snapshot is written, then restored to their original position. If it is set to *no* they will not be. The *no* setting is the default because it requires no extra computation.

The *precision* keyword only applies to the dump *xtc* style. A specified value of N means that coordinates are stored to 1/N nanometer accuracy, e.g. for N = 1000, the coordinates are written to 1/1000 nanometer accuracy.

The *refresh* keyword only applies to the dump *custom*, *cfg*, *image*, and *movie* styles. It allows an "incremental" dump file to be written, by refreshing a compute that is used as a threshold for determining which atoms are included in a dump snapshot. The specified *c_ID* gives the ID of the compute. It is prefixed by "c_" to indicate a compute, which is the only current option. At some point, other options may be added, e.g. fixes or variables.

Note: This keyword can only be specified once for a dump. Refreshes of multiple computes cannot yet be performed.

The definition and motivation of an incremental dump file is as follows. Instead of outputting all atoms at each snapshot (with some associated values), you may only wish to output the subset of atoms with a value that has changed in some way compared to the value the last time that atom was output. In some scenarios this can result in a dramatically smaller dump file. If desired, by post-processing the sequence of snapshots, the values for all atoms at all timesteps can be inferred.

A concrete example is a simulation of atom diffusion in a solid, represented as atoms on a lattice. Diffusive hops are rare. Imagine that when a hop occurs an atom moves more than a distance *Dhop*. For any snapshot we only want to output atoms that have hopped since the last snapshot. This can be accomplished with something the following commands:

```
variable        Dhop equal 0.6
variable        check atom "c_dsp[4] > v_Dhop"
compute         dsp all displace/atom refresh check
dump            1 all custom 20 tmp.dump id type x y z
dump_modify     1 append yes thresh c_dsp[4] > ${Dhop} refresh c_dsp
```

The *compute displace/atom* command calculates the displacement of each atom from its reference position. The "4" index is the scalar displacement; 1,2,3 are the xyz components of the displacement. The *dump_modify thresh* command will cause only atoms that have displaced more than 0.6 Angstroms to be output on a given snapshot (assuming metal units). However, note that when an atom is output, we also need to update the reference position for that atom to its new coordinates. So that it will not be output in every snapshot thereafter. That reference position is stored by *compute displace/atom*. So the dump_modify *refresh* option triggers a call to compute displace/atom at the end of every dump to perform that update. The *refresh check* option shown as part of the *compute displace/atom* command enables the compute to respond to the call from the dump command, and update the appropriate reference positions. This is done be defining an *atom-style variable*, *check* in this example, which calculates a Boolean value (0 or 1) for each atom, based on the same criterion used by dump_modify thresh.

See the *compute displace/atom* command for more details, including an example of how to produce output that includes an initial snapshot with the reference position of all atoms.

Note that only computes with a *refresh* option will work with dump_modify refresh. See individual compute doc pages for details. Currently, only compute displace/atom supports this option. Others may be added at some point. If you use a compute that doesn't support refresh operations, LAMMPS will not complain; dump_modify refresh will simply do nothing.

The *region* keyword only applies to the dump *custom*, *cfg*, *image*, and *movie* styles. If specified, only atoms in the region will be written to the dump file or included in the image/movie. Only one region can be applied as a filter (the last one specified). See the *region* command for more details. Note that a region can be defined as the "inside" or "outside" of a geometric shape, and it can be the "union" or "intersection" of a series of simpler regions.

The *scale* keyword applies only to the dump *atom* style. A scale value of *yes* means atom coords are written in normalized units from 0.0 to 1.0 in each box dimension. If the simulation box is triclinic (tilted), then all atom coords

will still be between 0.0 and 1.0. A value of *no* means they are written in absolute distance units (e.g. Angstroms or sigma).

The *sfactor* and *tfactor* keywords only apply to the dump *xtc* style. They allow customization of the unit conversion factors used when writing to XTC files. By default they are initialized for whatever *units* style is being used, to write out coordinates in nanometers and time in picoseconds. I.e. for *real* units, LAMMPS defines *sfactor* = 0.1 and *tfactor* = 0.001, since the Angstroms and fmsec used by *real* units are 0.1 nm and 0.001 psec respectively. If you are using a units system with distance and time units far from nm and psec, you may wish to write XTC files with different units, since the compression algorithm used in XTC files is most effective when the typical magnitude of position data is between 10.0 and 0.1.

The *sort* keyword determines whether lines of per-atom output in a snapshot are sorted or not. A sort value of *off* means they will typically be written in indeterminate order, either in serial or parallel. This is the case even in serial if the *atom_modify sort* option is turned on, which it is by default, to improve performance. A sort value of *id* means sort the output by atom ID. A sort value of N or -N means sort the output by the value in the Nth column of per-atom info in either ascending or descending order.

The dump *local* style cannot be sorted by atom ID, since there are typically multiple lines of output per atom. Some dump styles, such as *dcd* and *xtc*, require sorting by atom ID to format the output file correctly. If multiple processors are writing the dump file, via the "%" wildcard in the dump filename, then sorting cannot be performed.

Note: Unless it is required by the dump style, sorting dump file output requires extra overhead in terms of CPU and communication cost, as well as memory, versus unsorted output.

The *thermo* keyword only applies the dump *netcdf* style. It triggers writing of *thermo* information to the dump file alongside per-atom data. The values included in the dump file are identical to the values specified by *thermo_style*.

The *thresh* keyword only applies to the dump *custom*, *cfg*, *image*, and *movie* styles. Multiple thresholds can be specified. Specifying *none* turns off all threshold criteria. If thresholds are specified, only atoms whose attributes meet all the threshold criteria are written to the dump file or included in the image. The possible attributes that can be tested for are the same as those that can be specified in the *dump custom* command, with the exception of the *element* attribute, since it is not a numeric value. Note that a different attributes can be used than those output by the *dump custom* command. E.g. you can output the coordinates and stress of atoms whose energy is above some threshold.

If an atom-style variable is used as the attribute, then it can produce continuous numeric values or effective Boolean 0/1 values which may be useful for the comparison operator. Boolean values can be generated by variable formulas that use comparison or Boolean math operators or special functions like gmask() and rmask() and grmask(). See the *variable* command doc page for details.

The specified value must be a simple numeric value or the word LAST. If LAST is used, it refers to the value of the attribute the last time the dump command was invoked to produce a snapshot. This is a way to only dump atoms whose attribute has changed (or not changed). Three examples follow.

```
dump_modify ... thresh ix != LAST
```

This will dump atoms which have crossed the periodic x boundary of the simulation box since the last dump. (Note that atoms that crossed once and then crossed back between the two dump timesteps would not be included.)

```
region foo sphere 10 20 10 15
variable inregion atom rmask(foo)
dump_modify ... thresh v_inregion |^ LAST
```

This will dump atoms which crossed the boundary of the spherical region since the last dump.

```
variable charge atom "(q > 0.5) || (q < -0.5)"
dump_modify ... thresh v_charge |^ LAST
```

This will dump atoms whose charge has changed from an absolute value less than 1/2 to greater than 1/2 (or vice versa) since the last dump. E.g. due to reactions and subsequent charge equilibration in a reactive force field.

The choice of operators listed above are the usual comparison operators. The XOR operation (exclusive or) is also included as "|^". In this context, XOR means that if either the attribute or value is 0.0 and the other is non-zero, then the result is "true" and the threshold criterion is met. Otherwise it is not met.

The *time* keyword only applies to the dump *atom*, *custom*, and *local* styles (and their COMPRESS package versions *atom/gz*, *custom/gz* and *local/gz*). If set to *yes*, each frame will will contain two extra lines before the "ITEM: TIMESTEP" entry:

```
ITEM: TIME
<elapsed time>
```

This will output the current elapsed simulation time in current time units equivalent to the *thermo keyword time*. This is to simplify post-processing of trajectories using a variable time step, e.g. when using *fix dt/reset*. The default setting is *no*.

The *units* keyword only applies to the dump *atom*, *custom*, and *local* styles (and their COMPRESS package versions *atom/gz*, *custom/gz* and *local/gz*). If set to *yes*, each individual dump file will contain two extra lines at the very beginning with:

```
ITEM: UNITS
<units style>
```

This will output the current selected *units* style to the dump file and thus allows visualization and post-processing tools to determine the choice of units of the data in the dump file. The default setting is *no*.

The *unwrap* keyword only applies to the dump *dcd* and *xtc* styles. If set to *yes*, coordinates will be written "unwrapped" by the image flags for each atom. Unwrapped means that if the atom has passed through a periodic boundary one or more times, the value is printed for what the coordinate would be if it had not been wrapped back into the periodic box. Note that these coordinates may thus be far outside the box size stored with the snapshot.

These keywords apply only to the *dump image* and *dump movie* styles. Any keyword that affects an image, also affects a movie, since the movie is simply a collection of images. Some of the keywords only affect the *dump movie* style. The descriptions give details.

The *acolor* keyword can be used with the *dump image* command, when its atom color setting is *type*, to set the color that atoms of each type will be drawn in the image.

The specified *type* should be an integer from 1 to Ntypes = the number of atom types. A wildcard asterisk can be used in place of or in conjunction with the *type* argument to specify a range of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

The specified *color* can be a single color which is any of the 140 pre-defined colors (see below) or a color name defined by the dump_modify color option. Or it can be two or more colors separated by a "/" character, e.g. red/green/blue. In

the former case, that color is assigned to all the specified atom types. In the latter case, the list of colors are assigned in a round-robin fashion to each of the specified atom types.

The *adiam* keyword can be used with the *dump image* command, when its atom diameter setting is *type*, to set the size that atoms of each type will be drawn in the image. The specified *type* should be an integer from 1 to Ntypes. As with the *acolor* keyword, a wildcard asterisk can be used as part of the *type* argument to specify a range of atom types. The specified *diam* is the size in whatever distance *units* the input script is using, e.g. Angstroms.

The *amap* keyword can be used with the *dump image* command, with its *atom* keyword, when its atom setting is an atom-attribute, to setup a color map. The color map is used to assign a specific RGB (red/green/blue) color value to an individual atom when it is drawn, based on the atom's attribute, which is a numeric value, e.g. its x-component of velocity if the atom-attribute "vx" was specified.

The basic idea of a color map is that the atom-attribute will be within a range of values, and that range is associated with a series of colors (e.g. red, blue, green). An atom's specific value (vx = -3.2) can then mapped to the series of colors (e.g. halfway between red and blue), and a specific color is determined via an interpolation procedure.

There are many possible options for the color map, enabled by the *amap* keyword. Here are the details.

The *lo* and *hi* settings determine the range of values allowed for the atom attribute. If numeric values are used for *lo* and/or *hi*, then values that are lower/higher than that value are set to the value. I.e. the range is static. If *lo* is specified as *min* or *hi* as *max* then the range is dynamic, and the lower and/or upper bound will be calculated each time an image is drawn, based on the set of atoms being visualized.

The *style* setting is two letters, such as "ca". The first letter is either "c" for continuous, "d" for discrete, or "s" for sequential. The second letter is either "a" for absolute, or "f" for fractional.

A continuous color map is one in which the color changes continuously from value to value within the range. A discrete color map is one in which discrete colors are assigned to sub-ranges of values within the range. A sequential color map is one in which discrete colors are assigned to a sequence of sub-ranges of values covering the entire range.

An absolute color map is one in which the values to which colors are assigned are specified explicitly as values within the range. A fractional color map is one in which the values to which colors are assigned are specified as a fractional portion of the range. For example if the range is from -10.0 to 10.0, and the color red is to be assigned to atoms with a value of 5.0, then for an absolute color map the number 5.0 would be used. But for a fractional map, the number 0.75 would be used since 5.0 is 3/4 of the way from -10.0 to 10.0.

The *delta* setting must be specified for all styles, but is only used for the sequential style; otherwise the value is ignored. It specifies the bin size to use within the range for assigning consecutive colors to. For example, if the range is from -10.0 to 10.0 and a *delta* of 1.0 is used, then 20 colors will be assigned to the range. The first will be from -10.0 <= color1 < -9.0, then 2nd from -9.0 <= color2 < -8.0, etc.

The *N* setting is how many entries follow. The format of the entries depends on whether the color map style is continuous, discrete or sequential. In all cases the *color* setting can be any of the 140 pre-defined colors (see below) or a color name defined by the dump_modify color option.

For continuous color maps, each entry has a *value* and a *color*. The *value* is either a number within the range of values or *min* or *max*. The *value* of the first entry must be *min* and the *value* of the last entry must be *max*. Any entries in between must have increasing values. Note that numeric values can be specified either as absolute numbers or as fractions (0.0 to 1.0) of the range, depending on the "a" or "f" in the style setting for the color map.

Here is how the entries are used to determine the color of an individual atom, given the value X of its atom attribute. X will fall between 2 of the entry values. The color of the atom is linearly interpolated (in each of the RGB values) between the 2 colors associated with those entries. For example, if X = -5.0 and the 2 surrounding entries are "red" at -10.0 and "blue" at 0.0, then the atom's color will be halfway between "red" and "blue", which happens to be "purple".

For discrete color maps, each entry has a *lo* and *hi* value and a *color*. The *lo* and *hi* settings are either numbers within the range of values or *lo* can be *min* or *hi* can be *max*. The *lo* and *hi* settings of the last entry must be *min* and *max*.

Other entries can have any *lo* and *hi* values and the sub-ranges of different values can overlap. Note that numeric *lo* and *hi* values can be specified either as absolute numbers or as fractions (0.0 to 1.0) of the range, depending on the "a" or "f" in the style setting for the color map.

Here is how the entries are used to determine the color of an individual atom, given the value X of its atom attribute. The entries are scanned from first to last. The first time that *lo* <= X <= *hi*, X is assigned the color associated with that entry. You can think of the last entry as assigning a default color (since it will always be matched by X), and the earlier entries as colors that override the default. Also note that no interpolation of a color RGB is done. All atoms will be drawn with one of the colors in the list of entries.

For sequential color maps, each entry has only a *color*. Here is how the entries are used to determine the color of an individual atom, given the value X of its atom attribute. The range is partitioned into N bins of width *binsize*. Thus X will fall in a specific bin from 1 to N, say the Mth bin. If it falls on a boundary between 2 bins, it is considered to be in the higher of the 2 bins. Each bin is assigned a color from the E entries. If E < N, then the colors are repeated. For example if 2 entries with colors red and green are specified, then the odd numbered bins will be red and the even bins green. The color of the atom is the color of its bin. Note that the sequential color map is really a shorthand way of defining a discrete color map without having to specify where all the bin boundaries are.

Here is an example of using a sequential color map to color all the atoms in individual molecules with a different color. See the examples/pour/in.pour.2d.molecule input script for an example of how this is used.

```
variable        colors string &
                "red green blue yellow white &
                purple pink orange lime gray"
variable        mol atom mol%10
dump            1 all image 250 image.*.jpg v_mol type &
                zoom 1.6 adiam 1.5
dump_modify     1 pad 5 amap 0 10 sa 1 10 ${colors}
```

In this case, 10 colors are defined, and molecule IDs are mapped to one of the colors, even if there are 1000s of molecules.

The *backcolor* sets the background color of the images. The color name can be any of the 140 pre-defined colors (see below) or a color name defined by the dump_modify color option.

The *bcolor* keyword can be used with the *dump image* command, with its *bond* keyword, when its color setting is *type*, to set the color that bonds of each type will be drawn in the image.

The specified *type* should be an integer from 1 to Nbondtypes = the number of bond types. A wildcard asterisk can be used in place of or in conjunction with the *type* argument to specify a range of bond types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of bond types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

The specified *color* can be a single color which is any of the 140 pre-defined colors (see below) or a color name defined by the dump_modify color option. Or it can be two or more colors separated by a "/" character, e.g. red/green/blue. In the former case, that color is assigned to all the specified bond types. In the latter case, the list of colors are assigned in a round-robin fashion to each of the specified bond types.

The *bdiam* keyword can be used with the *dump image* command, with its *bond* keyword, when its diam setting is *type*, to set the diameter that bonds of each type will be drawn in the image. The specified *type* should be an integer from 1 to Nbondtypes. As with the *bcolor* keyword, a wildcard asterisk can be used as part of the *type* argument to specify a range of bond types. The specified *diam* is the size in whatever distance *units* you are using, e.g. Angstroms.

The *bitrate* keyword can be used with the *dump movie* command to define the size of the resulting movie file and its quality via setting how many kbits per second are to be used for the movie file. Higher bitrates require less compression and will result in higher quality movies. The quality is also determined by the compression format and encoder. The default setting is 2000 kbit/s, which will result in average quality with older compression formats.

Note: Not all movie file formats supported by dump movie allow the bitrate to be set. If not, the setting is silently ignored.

The *boxcolor* keyword sets the color of the simulation box drawn around the atoms in each image as well as the color of processor sub-domain boundaries. See the "dump image box" command for how to specify that a box be drawn via the *box* keyword, and the sub-domain boundaries via the *subbox* keyword. The color name can be any of the 140 pre-defined colors (see below) or a color name defined by the dump_modify color option.

The *color* keyword allows definition of a new color name, in addition to the 140-predefined colors (see below), and associates 3 red/green/blue RGB values with that color name. The color name can then be used with any other dump_modify keyword that takes a color name as a value. The RGB values should each be floating point values between 0.0 and 1.0 inclusive.

When a color name is converted to RGB values, the user-defined color names are searched first, then the 140 pre-defined color names. This means you can also use the *color* keyword to overwrite one of the pre-defined color names with new RBG values.

The *framerate* keyword can be used with the *dump movie* command to define the duration of the resulting movie file. Movie files written by the dump *movie* command have a default frame rate of 24 frames per second and the images generated will be converted at that rate. Thus a sequence of 1000 dump images will result in a movie of about 42 seconds. To make a movie run longer you can either generate images more frequently or lower the frame rate. To speed a movie up, you can do the inverse. Using a frame rate higher than 24 is not recommended, as it will result in simply dropping the rendered images. It is more efficient to dump images less frequently.

15.42.4 Restrictions

none

15.42.5 Related commands

dump, *dump image*, *undump*

15.42.6 Default

The option defaults are

- append = no
- buffer = yes for dump styles *atom*, *custom*, *loca*, and *xyz*
- element = "C" for every atom type

- every = whatever it was set to via the *dump* command
- fileper = # of processors
- first = no
- flush = yes
- format = %d and %g for each integer or floating point value
- image = no
- label = ENTRIES
- maxfiles = -1
- nfile = 1
- pad = 0
- pbc = no
- precision = 1000
- region = none
- scale = yes
- sort = off for dump styles *atom*, *custom*, *cfg*, and *local*
- sort = id for dump styles *dcd*, *xtc*, and *xyz*
- thresh = none
- units = no
- unwrap = no
- acolor = * red/green/blue/yellow/aqua/cyan
- adiam = * 1.0
- amap = min max cf 0.0 2 min blue max red
- backcolor = black
- bcolor = * red/green/blue/yellow/aqua/cyan
- bdiam = * 0.5
- bitrate = 2000
- boxcolor = yellow
- color = 140 color names are pre-defined as listed below
- framerate = 24

These are the standard 109 element names that LAMMPS pre-defines for use with the *dump image* and dump_modify commands.

- 1-10 = “H”, “He”, “Li”, “Be”, “B”, “C”, “N”, “O”, “F”, “Ne”
- 11-20 = “Na”, “Mg”, “Al”, “Si”, “P”, “S”, “Cl”, “Ar”, “K”, “Ca”
- 21-30 = “Sc”, “Ti”, “V”, “Cr”, “Mn”, “Fe”, “Co”, “Ni”, “Cu”, “Zn”
- 31-40 = “Ga”, “Ge”, “As”, “Se”, “Br”, “Kr”, “Rb”, “Sr”, “Y”, “Zr”

- 41-50 = “Nb”, “Mo”, “Tc”, “Ru”, “Rh”, “Pd”, “Ag”, “Cd”, “In”, “Sn”
- 51-60 = “Sb”, “Te”, “I”, “Xe”, “Cs”, “Ba”, “La”, “Ce”, “Pr”, “Nd”
- 61-70 = “Pm”, “Sm”, “Eu”, “Gd”, “Tb”, “Dy”, “Ho”, “Er”, “Tm”, “Yb”
- 71-80 = “Lu”, “Hf”, “Ta”, “W”, “Re”, “Os”, “Ir”, “Pt”, “Au”, “Hg”
- 81-90 = “Tl”, “Pb”, “Bi”, “Po”, “At”, “Rn”, “Fr”, “Ra”, “Ac”, “Th”
- 91-100 = “Pa”, “U”, “Np”, “Pu”, “Am”, “Cm”, “Bk”, “Cf”, “Es”, “Fm”
- 101-109 = “Md”, “No”, “Lr”, “Rf”, “Db”, “Sg”, “Bh”, “Hs”, “Mt”

These are the 140 colors that LAMMPS pre-defines for use with the *dump image* and dump_modify commands. Additional colors can be defined with the dump_modify color command. The 3 numbers listed for each name are the RGB (red/green/blue) values. Divide each value by 255 to get the equivalent 0.0 to 1.0 value.

aliceblue = 240, 248, 255	antiquewhite = 250, 235, 215	aqua = 0, 255, 255	aquamarine = 127, 255, 212	azure = 240, 255, 255
beige = 245, 245, 220	bisque = 255, 228, 196	black = 0, 0, 0	blanchedalmond = 255, 255, 205	blue = 0, 0, 255
blueviolet = 138, 43, 226	brown = 165, 42, 42	burlywood = 222, 184, 135	cadetblue = 95, 158, 160	chartreuse = 127, 255, 0
chocolate = 210, 105, 30	coral = 255, 127, 80	cornflowerblue = 100, 149, 237	cornsilk = 255, 248, 220	crimson = 220, 20, 60
cyan = 0, 255, 255	darkblue = 0, 0, 139	darkcyan = 0, 139, 139	darkgoldenrod = 184, 134, 11	darkgray = 169, 169, 169
darkgreen = 0, 100, 0	darkkhaki = 189, 183, 107	darkmagenta = 139, 0, 139	darkolivegreen = 85, 107, 47	darkorange = 255, 140, 0
darkorchid = 153, 50, 204	darkred = 139, 0, 0	darksalmon = 233, 150, 122	darkseagreen = 143, 188, 143	darkslateblue = 72, 61, 139
darkslategray = 47, 79, 79	darkturquoise = 0, 206, 209	darkviolet = 148, 0, 211	deeppink = 255, 20, 147	deepskyblue = 0, 191, 255
dimgray = 105, 105, 105	dodgerblue = 30, 144, 255	firebrick = 178, 34, 34	floralwhite = 255, 250, 240	forestgreen = 34, 139, 34
fuchsia = 255, 0, 255	gainsboro = 220, 220, 220	ghostwhite = 248, 248, 255	gold = 255, 215, 0	goldenrod = 218, 165, 32
gray = 128, 128, 128	green = 0, 128, 0	greenyellow = 173, 255, 47	honeydew = 240, 255, 240	hotpink = 255, 105, 180
indianred = 205, 92, 92	indigo = 75, 0, 130	ivory = 255, 240, 240	khaki = 240, 230, 140	lavender = 230, 230, 250
lavenderblush = 255, 240, 245	lawngreen = 124, 252, 0	lemonchiffon = 255, 250, 205	lightblue = 173, 216, 230	lightcoral = 240, 128, 128
lightcyan = 224, 255, 255	lightgoldenrodyellow = 250, 250, 210	lightgreen = 144, 238, 144	lightgrey = 211, 211, 211	lightpink = 255, 182, 193
lightsalmon = 255, 160, 122	lightseagreen = 32, 178, 170	lightskyblue = 135, 206, 250	lightslategray = 119, 136, 153	lightsteelblue = 176, 196, 222
lightyellow = 255, 255, 224	lime = 0, 255, 0	limegreen = 50, 205, 50	linen = 250, 240, 230	magenta = 255, 0, 255
maroon = 128, 0, 0	mediumaquamarine = 102, 205, 170	mediumblue = 0, 0, 205	mediumorchid = 186, 85, 211	mediumpurple = 147, 112, 219
mediumseagreen = 60, 179, 113	mediumslateblue = 123, 104, 238	mediumspringgreen = 0, 250, 154	mediumturquoise = 72, 209, 204	mediumvioletred = 199, 21, 133
midnightblue = 25, 25, 112	mintcream = 245, 255, 250	mistyrose = 255, 228, 225	moccasin = 255, 228, 181	navajowhite = 255, 222, 173
navy = 0, 0, 128	oldlace = 253, 245, 230	olive = 128, 128, 0	olivedrab = 107, 142, 35	orange = 255, 165, 0
orangered = 255, 69, 0	orchid = 218, 112, 214	palegoldenrod = 238, 232, 170	palegreen = 152, 251, 152	paleturquoise = 175, 238, 238
palevioletred = 219, 112, 147	papayawhip = 255, 239, 213	peachpuff = 255, 239, 213	peru = 205, 133, 63	pink = 255, 192, 203
plum = 221, 160, 221	powderblue = 176, 224, 230	purple = 128, 0, 128	red = 255, 0, 0	rosybrown = 188, 143, 143
royalblue = 65, 105, 225	saddlebrown = 139, 69, 19	salmon = 250, 128, 114	sandybrown = 244, 164, 96	seagreen = 46, 139, 87
seashell = 255, 245, 238	sienna = 160, 82, 45	silver = 192, 192, 192	skyblue = 135, 206, 235	slateblue = 106, 90, 205
slategray = 112, 128, 144	snow = 255, 250, 250	springgreen = 0, 255, 127	steelblue = 70, 130, 180	tan = 210, 180, 140
teal = 0, 128, 128	thistle = 216, 191, 216	tomato = 253, 99, 71	turquoise = 64, 224, 208	violet = 238, 130, 238
wheat = 245, 222, 179	white = 255, 255, 255	whitesmoke = 245, 245, 245	yellow = 255, 255, 0	yellowgreen = 154, 205, 50

15.43 dump molfile command

15.43.1 Syntax

```
dump ID group-ID molfile N file format path
```

- ID = user-assigned name for the dump
- group-ID = ID of the group of atoms to be imaged
- molfile = style of dump command (other styles *atom* or *cfg* or *dcd* or *xtc* or *xyz* or *local* or *custom* are discussed on the *dump* doc page)
- N = dump every this many timesteps
- file = name of file to write to
- format = file format to be used
- path = file path with plugins (optional)

15.43.2 Examples

```
dump mf1 all molfile 10 melt1.xml hoomd
dump mf2 all molfile 10 melt2-*.pdb pdb .
dump mf3 all molfile 50 melt3.xyz xyz .:/home/akohlmey/vmd/plugins/LINUX/
↪molfile
```

15.43.3 Description

Dump a snapshot of atom coordinates and selected additional quantities to one or more files every N timesteps in one of several formats. Only information for atoms in the specified group is dumped. This specific dump style uses molfile plugins that are bundled with the VMD molecular visualization and analysis program.

Unless the filename contains a * character, the output will be written to one single file with the specified format. Otherwise there will be one file per snapshot and the * will be replaced by the time step number when the snapshot is written.

Note: Because periodic boundary conditions are enforced only on timesteps when neighbor lists are rebuilt, the coordinates of an atom written to a dump file may be slightly outside the simulation box.

The molfile plugin API has a few restrictions that have to be honored by this dump style: the number of atoms must not change, the atoms must be sorted, outside of the coordinates no change in atom properties (like type, mass, charge) will be recorded.

The *format* keyword determines what format is used to write out the dump. For this to work, LAMMPS must be able to find and load a compatible molfile plugin that supports this format. Settings made via the *dump_modify* command can alter per atom properties like element names.

The *path* keyword determines which in directories. This is a "path" like other search paths, i.e. it can contain multiple directories separated by a colon (or semi-colon on windows). This keyword is optional and default to ".", the current directory.

The *unwrap* option of the *dump_modify* command allows coordinates to be written "unwrapped" by the image flags for each atom. Unwrapped means that if the atom has passed through a periodic boundary one or more times, the value is printed for what the coordinate would be if it had not been wrapped back into the periodic box. Note that these coordinates may thus be far outside the box size stored with the snapshot.

Dumps are performed on timesteps that are a multiple of N (including timestep 0) and on the last timestep of a minimization if the minimization converges. Note that this means a dump will not be performed on the initial timestep after the dump command is invoked, if the current timestep is not a multiple of N. This behavior can be changed via the *dump_modify first* command, which can be useful if the dump command is invoked after a minimization ended on an arbitrary timestep. N can be changed between runs by using the *dump_modify every* command. The *dump_modify every* command also allows a variable to be used to determine the sequence of timesteps on which dump files are written.

15.43.4 Restrictions

The *molfile* dump style is part of the USER-MOLFILE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Molfile plugins provide a consistent programming interface to read and write file formats commonly used in molecular simulations. The USER-MOLFILE package only provides the interface code, not the plugins. These can be obtained from a VMD installation which has to match the platform that you are using to compile LAMMPS for. By adding plugins to VMD, support for new file formats can be added to LAMMPS (or VMD or other programs that use them) without having to re-compile the application itself. The plugins are installed in the directory: <VMDHOME>/plugins/<VMDARCH>/molfile

---

Note: while the programming interface (API) to the plugins is backward compatible, the binary interface (ABI) has been changing over time, so it is necessary to compile this package with the plugin header files from VMD that match the binary plugins. These header files in the directory: <VMDHOME>/plugins/include For convenience, the package ships with a set of header files that are compatible with VMD 1.9 and 1.9.1 (June 2012)

15.43.5 Related commands

dump, *dump_modify*, *undump*

15.43.6 Default

The default path is ".". All other properties have to be specified.

15.44 dump netcdf command

15.45 dump netcdf/mpiio command

15.45.1 Syntax

```
dump ID group-ID netcdf N file args
dump ID group-ID netcdf/mpiio N file args
```

- ID = user-assigned name for the dump
- group-ID = ID of the group of atoms to be imaged
- *netcdf* or *netcdf/mpiio* = style of dump command (other styles *atom* or *cfg* or *dcd* or *xtc* or *xyz* or *local* or *custom* are discussed on the *dump* doc page)
- N = dump every this many timesteps
- file = name of file to write dump info to
- args = list of atom attributes, same as for *dump_style custom*

15.45.2 Examples

```
dump 1 all netcdf 100 traj.nc type x y z vx vy vz
dump_modify 1 append yes at -1 thermo yes
dump 1 all netcdf/mpiio 1000 traj.nc id type x y z
dump 1 all netcdf 1000 traj.*.nc id type x y z
```

15.45.3 Description

Dump a snapshot of atom coordinates every N timesteps in Amber-style NetCDF file format. NetCDF files are binary, portable and self-describing. This dump style will write only one file on the root node. The dump style *netcdf* uses the standard NetCDF library. All data is collected on one processor and then written to the dump file. Dump style *netcdf/mpiio* uses the parallel NetCDF library and MPI-IO to write to the dump file in parallel; it has better performance on a larger number of processors. Note that style *netcdf* outputs all atoms sorted by atom tag while style *netcdf/mpiio* outputs atoms in order of their MPI rank.

NetCDF files can be directly visualized via the following tools:

Ovito (http://www.ovito.org/). Ovito supports the AMBER convention and all extensions of this dump style.

- VMD (http://www.ks.uiuc.edu/Research/vmd/).
- AtomEye (http://www.libatoms.org/). The libAtoms version of AtomEye contains a NetCDF reader that is not present in the standard distribution of AtomEye.

In addition to per-atom data, *thermo* data can be included in the dump file. The data included in the dump file is identical to the data specified by *thermo_style*.

15.45.4 Restrictions

The *netcdf* and *netcdf/mpiio* dump styles are part of the USER-NETCDF package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

15.45.5 Related commands

dump, *dump_modify*, *undump*

15.46 dump vtk command

15.46.1 Syntax

```
dump ID group-ID vtk N file args
```

- ID = user-assigned name for the dump
- group-ID = ID of the group of atoms to be dumped
- vtk = style of dump command (other styles *atom* or *cfg* or *dcd* or *xtc* or *xyz* or *local* or *custom* are discussed on the *dump* doc page)
- N = dump every this many timesteps
- file = name of file to write dump info to
- args = same as arguments for *dump_style custom*

15.46.2 Examples

```
dump dmpvtk all vtk 100 dump*.myforce.vtk id type vx fx
dump dmpvtp flow vtk 100 dump*.%.displace.vtp id type c_myD[1] c_myD[2] c_
↪myD[3] v_ke
```

15.46.3 Description

Dump a snapshot of atom quantities to one or more files every N timesteps in a format readable by the VTK visualization toolkit or other visualization tools that use it, e.g. ParaView. The timesteps on which dump output is written can also be controlled by a variable; see the *dump_modify every* command for details.

This dump style is similar to *dump_style custom* but uses the VTK library to write data to VTK simple legacy or XML format depending on the filename extension specified for the dump file. This can be either **.vtk* for the legacy format or **.vtp* and **.vtu*, respectively, for XML format; see the VTK homepage for a detailed description of these formats. Since this naming convention conflicts with the way binary output is usually specified (see below), the *dump_modify binary* command allows setting of a binary option for this dump style explicitly.

Only information for atoms in the specified group is dumped. The *dump_modify thresh and region* commands can also alter what atoms are included; see details below.

As described below, special characters ("*", "%") in the filename determine the kind of output.

Warning: Because periodic boundary conditions are enforced only on timesteps when neighbor lists are rebuilt, the coordinates of an atom written to a dump file may be slightly outside the simulation box.

Warning: Unless the *dump_modify sort* option is invoked, the lines of atom information written to dump files will be in an indeterminate order for each snapshot. This is even true when running on a single processor, if the *atom_modify sort* option is on, which it is by default. In this case atoms are re-ordered periodically during a simulation, due to spatial sorting. It is also true when running in parallel, because data for a single snapshot is collected from multiple processors, each of which owns a subset of the atoms.

For the *vtk* style, sorting is off by default. See the *dump_modify* doc page for details.

The dimensions of the simulation box are written to a separate file for each snapshot (either in legacy VTK or XML format depending on the format of the main dump file) with the suffix *_boundingBox* appended to the given dump filename.

For an orthogonal simulation box this information is saved as a rectilinear grid (legacy .vtk or .vtr XML format).

Triclinic simulation boxes (non-orthogonal) are saved as hexahedrons in either legacy .vtk or .vtu XML format.

Style *vtk* allows you to specify a list of atom attributes to be written to the dump file for each atom. The list of possible attributes is the same as for the *dump_style custom* command; see its doc page for a listing and an explanation of each attribute.

Note: Since position data is required to write VTK files the atom attributes "x y z" do not have to be specified explicitly; they will be included in the dump file regardless. Also, in contrast to the *custom* style, the specified *vtk* attributes are rearranged to ensure correct ordering of vector components (except for computes and fixes - these have to be given in the right order) and duplicate entries are removed.

The VTK format uses a single snapshot of the system per file, thus a wildcard "*" must be included in the filename, as discussed below. Otherwise the dump files will get overwritten with the new snapshot each time.

Dumps are performed on timesteps that are a multiple of N (including timestep 0) and on the last timestep of a minimization if the minimization converges. Note that this means a dump will not be performed on the initial timestep after the dump command is invoked, if the current timestep is not a multiple of N. This behavior can be changed via the *dump_modify first* command, which can also be useful if the dump command is invoked after a minimization ended on an arbitrary timestep. N can be changed between runs by using the *dump_modify every* command. The *dump_modify every* command also allows a variable to be used to determine the sequence of timesteps on which dump files are written. In this mode a dump on the first timestep of a run will also not be written unless the *dump_modify first* command is used.

Dump filenames can contain two wildcard characters. If a "*" character appears in the filename, then one file per snapshot is written and the "*" character is replaced with the timestep value. For example, tmp.dump*.vtk becomes tmp.dump0.vtk, tmp.dump10000.vtk, tmp.dump20000.vtk, etc. Note that the *dump_modify pad* command can be used to insure all timestep numbers are the same length (e.g. 00010), which can make it easier to read a series of dump files in order with some post-processing tools.

If a "%" character appears in the filename, then each of P processors writes a portion of the dump file, and the "%" character is replaced with the processor ID from 0 to P-1 preceded by an underscore character. For example, tmp.dump%.vtp becomes tmp.dump_0.vtp, tmp.dump_1.vtp, ... tmp.dump_P-1.vtp, etc. This creates smaller files and can be a fast mode of output on parallel machines that support parallel I/O for output.

By default, P = the number of processors meaning one file per processor, but P can be set to a smaller value via the *nfile* or *fileper* keywords of the *dump_modify* command. These options can be the most efficient way of writing out dump files when running on large numbers of processors.

For the legacy VTK format "%" is ignored and P = 1, i.e., only processor 0 does write files.

Note that using the "*" and "%" characters together can produce a large number of small dump files!

If *dump_modify binary* is used, the dump file (or files, if "*" or "%" is also used) is written in binary format. A binary dump file will be about the same size as a text version, but will typically write out much faster.

15.46.4 Restrictions

The *vtk* style does not support writing of gzipped dump files.

The *vtk* dump style is part of the USER-VTK package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

To use this dump style, you also must link to the VTK library. See the info in lib/vtk/README and insure the Makefile.lammps file in that directory is appropriate for your machine.

The *vtk* dump style supports neither buffering or custom format strings.

15.46.5 Related commands

dump, *dump image*, *dump_modify*, *undump*

15.46.6 Default

By default, files are written in ASCII format. If the file extension is not one of .vtk, .vtp or .vtu, the legacy VTK file format is used.

15.47 dynamical_matrix command

15.47.1 Syntax

```
dynamical_matrix group-ID style gamma args keyword value ...
```

- group-ID = ID of group of atoms to displace
- style = *regular* or *eskm*
- gamma = finite different displacement length (distance units)
- one or more keyword/arg pairs may be appended

```
keyword = file or binary
  file name = name of output file for the dynamical matrix
  binary arg = yes or no or gzip
```

15.47.2 Examples

```
dynamical_matrix 1 regular 0.000001
dynamical_matrix 1 eskm 0.000001
dynamical_matrix 3 regular 0.00004 file dynmat.dat
dynamical_matrix 5 eskm 0.00000001 file dynamical.dat binary yes
```

15.47.3 Description

Calculate the dynamical matrix by finite difference of the selected group,

$$D = \frac{\Phi_{ij}^{\alpha\beta}}{\sqrt{M_i M_j}}$$

where D is the dynamical matrix and Φ is the force constant matrix defined by

$$\Phi_{ij}^{\alpha\beta} = \frac{\partial^2 U}{\partial x_{i,\alpha} \partial x_{j,\beta}}$$

The output for the dynamical matrix is printed three elements at a time. The three elements are the three β elements for a respective i/α/j combination. Each line is printed in order of j increasing first, α second, and i last.

If the style eskm is selected, the dynamical matrix will be in units of inverse squared femtoseconds. These units will then conveniently leave frequencies in THz.

15.47.4 Restrictions

The command collects an array of nine times the number of atoms in a group on every single MPI rank, so the memory requirements can be very significant for large systems.

This command is part of the USER-PHONON package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

15.47.5 Related commands

fix phonon

compute hma uses an analytic formulation of the Hessian provided by a pair_style's Pair::single_hessian() function, if implemented.

15.47.6 Default

The default settings are file = "dynmat.dyn", binary = no

15.48 echo command

15.48.1 Syntax

```
echo style
```

- style = *none* or *screen* or *log* or *both*

15.48.2 Examples

```
echo both
echo log
```

15.48.3 Description

This command determines whether LAMMPS echoes each input script command to the screen and/or log file as it is read and processed. If an input script has errors, it can be useful to look at echoed output to see the last command processed.

The *command-line switch* -echo can be used in place of this command.

15.48.4 Restrictions

none

Related commands: none

15.48.5 Default

```
echo log
```

15.49 fix command

15.49.1 Syntax

```
fix ID group-ID style args
```

- ID = user-assigned name for the fix
- group-ID = ID of the group of atoms to apply the fix to
- style = one of a long list of possible style names (see below)
- args = arguments used by a particular style

15.49.2 Examples

```
fix 1 all nve
fix 3 all nvt temp 300.0 300.0 0.01
fix mine top setforce 0.0 NULL 0.0
```

15.49.3 Description

Set a fix that will be applied to a group of atoms. In LAMMPS, a "fix" is any operation that is applied to the system during timestepping or minimization. Examples include updating of atom positions and velocities due to time integration, controlling temperature, applying constraint forces to atoms, enforcing boundary conditions, computing diagnostics, etc. There are hundreds of fixes defined in LAMMPS and new ones can be added; see the *Modify* doc page for details.

Fixes perform their operations at different stages of the timestep. If 2 or more fixes operate at the same stage of the timestep, they are invoked in the order they were specified in the input script.

The ID of a fix can only contain alphanumeric characters and underscores.

Fixes can be deleted with the *unfix* command.

Note: The *unfix* command is the only way to turn off a fix; simply specifying a new fix with a similar style will not turn off the first one. This is especially important to realize for integration fixes. For example, using a *fix nve* command for a second run after using a *fix nvt* command for the first run, will not cancel out the NVT time integration invoked by the "fix nvt" command. Thus two time integrators would be in place!

If you specify a new fix with the same ID and style as an existing fix, the old fix is deleted and the new one is created (presumably with new settings). This is the same as if an "unfix" command were first performed on the old fix, except that the new fix is kept in the same order relative to the existing fixes as the old one originally was. Note that this operation also wipes out any additional changes made to the old fix via the *fix_modify* command.

The *fix modify* command allows settings for some fixes to be reset. See the doc page for individual fixes for details.

Some fixes store an internal "state" which is written to binary restart files via the *restart* or *write_restart* commands. This allows the fix to continue on with its calculations in a restarted simulation. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file. See the doc pages for individual fixes for info on which ones can be restarted.

Some fixes calculate one of three styles of quantities: global, per-atom, or local, which can be used by other commands or output as described below. A global quantity is one or more system-wide values, e.g. the energy of a wall interacting with particles. A per-atom quantity is one or more values per atom, e.g. the displacement vector for each atom since time 0. Per-atom values are set to 0.0 for atoms not in the specified fix group. Local quantities are calculated by each processor based on the atoms it owns, but there may be zero or more per atoms.

Note that a single fix can produce either global or per-atom or local quantities (or none at all), but not both global and per-atom. It can produce local quantities in tandem with global or per-atom quantities. The fix doc page will explain.

Global, per-atom, and local quantities each come in three kinds: a single scalar value, a vector of values, or a 2d array of values. The doc page for each fix describes the style and kind of values it produces, e.g. a per-atom vector. Some fixes produce more than one kind of a single style, e.g. a global scalar and a global vector.

When a fix quantity is accessed, as in many of the output commands discussed below, it can be referenced via the following bracket notation, where ID is the ID of the fix:

f_ID	entire scalar, vector, or array
f_ID[I]	one element of vector, one column of array
f_ID[I][J]	one element of array

In other words, using one bracket reduces the dimension of the quantity once (vector -> scalar, array -> vector). Using two brackets reduces the dimension twice (array -> scalar). Thus a command that uses scalar fix values as input can also process elements of a vector or array.

Note that commands and *variables* which use fix quantities typically do not allow for all kinds, e.g. a command may require a vector of values, not a scalar. This means there is no ambiguity about referring to a fix quantity as f_ID even if it produces, for example, both a scalar and vector. The doc pages for various commands explain the details.

In LAMMPS, the values generated by a fix can be used in several ways:

- Global values can be output via the *thermo_style custom* or *fix ave/time* command. Or the values can be referenced in a *variable equal* or *variable atom* command.
- Per-atom values can be output via the *dump custom* command. Or they can be time-averaged via the *fix ave/atom* command or reduced by the *compute reduce* command. Or the per-atom values can be referenced in an *atom-style variable*.
- Local values can be reduced by the *compute reduce* command, or histogrammed by the *fix ave/histo* command.

See the *Howto output* doc page for a summary of various LAMMPS output options, many of which involve fixes.

The results of fixes that calculate global quantities can be either "intensive" or "extensive" values. Intensive means the value is independent of the number of atoms in the simulation, e.g. temperature. Extensive means the value scales with the number of atoms in the simulation, e.g. total rotational kinetic energy. *Thermodynamic output* will normalize extensive values by the number of atoms in the system, depending on the "thermo_modify norm" setting. It will not normalize intensive values. If a fix value is accessed in another way, e.g. by a *variable*, you may want to know whether it is an intensive or extensive value. See the doc page for individual fixes for further info.

Each fix style has its own doc page which describes its arguments and what it does, as listed below. Here is an alphabetic list of fix styles available in LAMMPS. They are also listed in more compact form on the *Commands fix* doc page.

There are also additional accelerated fix styles included in the LAMMPS distribution for faster performance on CPUs, GPUs, and KNLs. The individual style names on the *Commands fix* doc page are followed by one or more of (g,i,k,o,t) to indicate which accelerated styles exist.

- *adapt* - change a simulation parameter over time
- *adapt/fep* - enhanced version of fix adapt
- *addforce* - add a force to each atom
- *addtorque* - add a torque to a group of atoms
- *append/atoms* - append atoms to a running simulation
- *atc* - initiates a coupled MD/FE simulation
- *atom/swap* - Monte Carlo atom type swapping
- *ave/atom* - compute per-atom time-averaged quantities
- *ave/chunk* - compute per-chunk time-averaged quantities
- *ave/correlate* - compute/output time correlations

- *ave/correlate/long* -
- *ave/histo* - compute/output time-averaged histograms
- *ave/histo/weight* - weighted version of fix ave/histo
- *ave/time* - compute/output global time-averaged quantities
- *aveforce* - add an averaged force to each atom
- *balance* - perform dynamic load-balancing
- *bocs* - NPT style time integration with pressure correction
- *bond/break* - break bonds on the fly
- *bond/create* - create bonds on the fly
- *bond/react* - apply topology changes to model reactions
- *bond/swap* - Monte Carlo bond swapping
- *box/relax* - relax box size during energy minimization
- *client/md* - MD client for client/server simulations
- *cmap* - enables CMAP cross-terms of the CHARMM force field
- *colvars* - interface to the collective variables "Colvars" library
- *controller* - apply control loop feedback mechanism
- *deform* - change the simulation box size/shape
- *deposit* - add new atoms above a surface
- *dpd/energy* - constant energy dissipative particle dynamics
- *drag* - drag atoms towards a defined coordinate
- *drude* - part of Drude oscillator polarization model
- *drude/transform/direct* - part of Drude oscillator polarization model
- *drude/transform/inverse* - part of Drude oscillator polarization model
- *dt/reset* - reset the timestep based on velocity, forces
- *edpd/source* - add heat source to eDPD simulations
- *efield* - impose electric field on system
- *ehex* - enhanced heat exchange algorithm
- *electron/stopping* - electronic stopping power as a friction force
- *enforce2d* - zero out z-dimension velocity and force
- *eos/cv* -
- *eos/table* -
- *eos/table/rx* -
- *evaporate* - remove atoms from simulation periodically
- *external* - callback to an external driver program
- *ffl* - apply a Fast-Forward Langevin equation thermostat
- *filter/corotate* - implement corotation filter to allow larger timesteps with r-RESPA

- *flow/gauss* - Gaussian dynamics for constant mass flux
- *freeze* - freeze atoms in a granular simulation
- *gcmc* - grand canonical insertions/deletions
- *gld* - generalized Langevin dynamics integrator
- *gle* - generalized Langevin equation thermostat
- *gravity* - add gravity to atoms in a granular simulation
- *grem* - implements the generalized replica exchange method
- *halt* - terminate a dynamics run or minimization
- *heat* - add/subtract momentum-conserving heat
- *hyper/global* - global hyperdynamics
- *hyper/local* - local hyperdynamics
- *imd* - implements the "Interactive MD" (IMD) protocol
- *indent* - impose force due to an indenter
- *ipi* - enable LAMMPS to run as a client for i-PI path-integral simulations
- *langevin* - Langevin temperature control
- *langevin/drude* - Langevin temperature control of Drude oscillators
- *langevin/eff* - Langevin temperature control for the electron force field model
- *langevin/spin* - Langevin temperature control for a spin or spin-lattice system
- *latte* - wrapper on LATTE density-functional tight-binding code
- *lb/fluid* -
- *lb/momentum* -
- *lb/pc* -
- *lb/rigid/pc/sphere* -
- *lb/viscous* -
- *lineforce* - constrain atoms to move in a line
- *manifoldforce* - restrain atoms to a manifold during minimization
- *meso* - time integration for SPH/DPDE particles
- *meso/move* - move mesoscopic SPH/SDPD particles in a prescribed fashion
- *meso/stationary* -
- *momentum* - zero the linear and/or angular momentum of a group of atoms
- *move* - move atoms in a prescribed fashion
- *mscg* - apply MSCG method for force-matching to generate coarse grain models
- *msst* - multi-scale shock technique (MSST) integration
- *mvv/dpd* - DPD using the modified velocity-Verlet integration algorithm
- *mvv/edpd* - constant energy DPD using the modified velocity-Verlet algorithm
- *mvv/tdpd* - constant temperature DPD using the modified velocity-Verlet algorithm

- *neb* - nudged elastic band (NEB) spring forces
- *neb/spin* - nudged elastic band (NEB) spring forces for spins
- *nph* - constant NPH time integration via Nose/Hoover
- *nph/asphere* - NPH for aspherical particles
- *nph/body* - NPH for body particles
- *nph/eff* - NPH for nuclei and electrons in the electron force field model
- *nph/sphere* - NPH for spherical particles
- *nphug* - constant-stress Hugoniostat integration
- *npt* - constant NPT time integration via Nose/Hoover
- *npt/asphere* - NPT for aspherical particles
- *npt/body* - NPT for body particles
- *npt/cauchy* - NPT with Cauchy stress
- *npt/eff* - NPT for nuclei and electrons in the electron force field model
- *npt/sphere* - NPT for spherical particles
- *npt/uef* - NPT style time integration with diagonal flow
- *nve* - constant NVE time integration
- *nve/asphere* - NVE for aspherical particles
- *nve/asphere/noforce* - NVE for aspherical particles without forces
- *nve/awpmd* - NVE for the Antisymmetrized Wave Packet Molecular Dynamics model
- *nve/body* - NVE for body particles
- *nve/dot* - rigid body constant energy time integrator for coarse grain models
- *nve/dotc/langevin* - Langevin style rigid body time integrator for coarse grain models
- *nve/eff* - NVE for nuclei and electrons in the electron force field model
- *nve/limit* - NVE with limited step length
- *nve/line* - NVE for line segments
- *nve/manifold/rattle* -
- *nve/noforce* - NVE without forces (v only)
- *nve/sphere* - NVE for spherical particles
- *nve/spin* - NVE for a spin or spin-lattice system
- *nve/tri* - NVE for triangles
- *nvk* - constant kinetic energy time integration
- *nvt* - NVT time integration via Nose/Hoover
- *nvt/asphere* - NVT for aspherical particles
- *nvt/body* - NVT for body particles
- *nvt/eff* - NVE for nuclei and electrons in the electron force field model
- *nvt/manifold/rattle* -

- *nvt/sllod* - NVT for NEMD with SLLOD equations
- *nvt/sllod/eff* - NVT for NEMD with SLLOD equations for the electron force field model
- *nvt/sphere* - NVT for spherical particles
- *nvt/uef* - NVT style time integration with diagonal flow
- *oneway* - constrain particles on move in one direction
- *orient/bcc* - add grain boundary migration force for BCC
- *orient/fcc* - add grain boundary migration force for FCC
- *phonon* - calculate dynamical matrix from MD simulations
- *pimd* - Feynman path integral molecular dynamics
- *planeforce* - constrain atoms to move in a plane
- *plumed* - wrapper on PLUMED free energy library
- *poems* - constrain clusters of atoms to move as coupled rigid bodies
- *pour* - pour new atoms/molecules into a granular simulation domain
- *precession/spin* -
- *press/berendsen* - pressure control by Berendsen barostat
- *print* - print text and variables during a simulation
- *propel/self* - model self-propelled particles
- *property/atom* - add customized per-atom values
- *python/invoke* - call a Python function during a simulation
- *python/move* - call a Python function during a simulation run
- *qbmsst* - quantum bath multi-scale shock technique time integrator
- *qeq/comb* - charge equilibration for COMB potential
- *qeq/dynamic* - charge equilibration via dynamic method
- *qeq/fire* - charge equilibration via FIRE minimizer
- *qeq/point* - charge equilibration via point method
- *qeq/reax* - charge equilibration for ReaxFF potential
- *qeq/shielded* - charge equilibration via shielded method
- *qeq/slater* - charge equilibration via Slater method
- *qmmm* - functionality to enable a quantum mechanics/molecular mechanics coupling
- *qtb* - implement quantum thermal bath scheme
- *rattle* - RATTLE constraints on bonds and/or angles
- *reax/c/bonds* - write out ReaxFF bond information
- *reax/c/species* - write out ReaxFF molecule information
- *recenter* - constrain the center-of-mass position of a group of atoms
- *restrain* - constrain a bond, angle, dihedral
- *rhok* - add bias potential for long-range ordered systems

- *rigid* - constrain one or more clusters of atoms to move as a rigid body with NVE integration
- *rigid/meso* - constrain clusters of mesoscopic SPH/SDPD particles to move as a rigid body
- *rigid/nph* - constrain one or more clusters of atoms to move as a rigid body with NPH integration
- *rigid/nph/small* - constrain many small clusters of atoms to move as a rigid body with NPH integration
- *rigid/npt* - constrain one or more clusters of atoms to move as a rigid body with NPT integration
- *rigid/npt/small* - constrain many small clusters of atoms to move as a rigid body with NPT integration
- *rigid/nve* - constrain one or more clusters of atoms to move as a rigid body with alternate NVE integration
- *rigid/nve/small* - constrain many small clusters of atoms to move as a rigid body with alternate NVE integration
- *rigid/nvt* - constrain one or more clusters of atoms to move as a rigid body with NVT integration
- *rigid/nvt/small* - constrain many small clusters of atoms to move as a rigid body with NVT integration
- *rigid/small* - constrain many small clusters of atoms to move as a rigid body with NVE integration
- *rx* -
- *saed/vtk* -
- *setforce* - set the force on each atom
- *setforce/spin* - set magnetic precession vectors on each atom
- *shake* - SHAKE constraints on bonds and/or angles
- *shardlow* - integration of DPD equations of motion using the Shardlow splitting
- *smd* - applied a steered MD force to a group
- *smd/adjust_dt* -
- *smd/integrate_tlsph* -
- *smd/integrate_ulsph* -
- *smd/move_tri_surf* -
- *smd/setvel* -
- *smd/wall_surface* -
- *spring* - apply harmonic spring force to group of atoms
- *spring/chunk* - apply harmonic spring force to each chunk of atoms
- *spring/rg* - spring on radius of gyration of group of atoms
- *spring/self* - spring from each atom to its origin
- *srd* - stochastic rotation dynamics (SRD)
- *store/force* - store force on each atom
- *store/state* - store attributes for each atom
- *tdpd/source* -
- *temp/berendsen* - temperature control by Berendsen thermostat
- *temp/csld* - canonical sampling thermostat with Langevin dynamics
- *temp/csvr* - canonical sampling thermostat with Hamiltonian dynamics
- *temp/rescale* - temperature control by velocity rescaling

- *temp/rescale/eff* - temperature control by velocity rescaling in the electron force field model
- *tfmc* - perform force-bias Monte Carlo with time-stamped method
- *thermal/conductivity* - Muller-Plathe kinetic energy exchange for thermal conductivity calculation
- *ti/spring* -
- *tmd* - guide a group of atoms to a new configuration
- *ttm* - two-temperature model for electronic/atomic coupling
- *ttm/mod* - enhanced two-temperature model with additional options
- *tune/kspace* - auto-tune KSpace parameters
- *vector* - accumulate a global vector every N timesteps
- *viscosity* - Muller-Plathe momentum exchange for viscosity calculation
- *viscous* - viscous damping for granular simulations
- *wall/body/polygon* -
- *wall/body/polyhedron* -
- *wall/colloid* - Lennard-Jones wall interacting with finite-size particles
- *wall/ees* - wall for ellipsoidal particles
- *wall/gran* - frictional wall(s) for granular simulations
- *wall/gran/region* -
- *wall/harmonic* - harmonic spring wall
- *wall/lj1043* - Lennard-Jones 10-4-3 wall
- *wall/lj126* - Lennard-Jones 12-6 wall
- *wall/lj93* - Lennard-Jones 9-3 wall
- *wall/morse* - Morse potential wall
- *wall/piston* - moving reflective piston wall
- *wall/reflect* - reflecting wall(s)
- *wall/reflect/stochastic* - reflecting wall(s) with finite temperature
- *wall/region* - use region surface as wall
- *wall/region/ees* - use region surface as wall for ellipsoidal particles
- *wall/srd* - slip/no-slip wall for SRD particles

15.49.4 Restrictions

Some fix styles are part of specific packages. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info. The doc pages for individual fixes tell if it is part of a package.

15.49.5 Related commands

unfix, *fix_modify*

Default: none

15.50 fix_modify command

15.50.1 Syntax

```
fix_modify fix-ID keyword value ...
```

- fix-ID = ID of the fix to modify
- one or more keyword/value pairs may be appended
- keyword = *temp* or *press* or *energy* or *virial* or *respa* or *dynamic/dof* or *bodyforces*

```
temp value = compute ID that calculates a temperature
press value = compute ID that calculates a pressure
energy value = yes or no
virial value = yes or no
respa value = 1 to max respa level or 0 (for outermost level)
dynamic/dof value = yes or no
  yes/no = do or do not re-compute the number of degrees of freedom (DOF)␣
↪contributing to the temperature
bodyforces value = early or late
  early/late = compute rigid-body forces/torques early or late in the␣
↪timestep
```

15.50.2 Examples

```
fix_modify 3 temp myTemp press myPress
fix_modify 1 energy yes
fix_modify tether respa 2
```

15.50.3 Description

Modify one or more parameters of a previously defined fix. Only specific fix styles support specific parameters. See the doc pages for individual fix commands for info on which ones support which fix_modify parameters.

The *temp* keyword is used to determine how a fix computes temperature. The specified compute ID must have been previously defined by the user via the *compute* command and it must be a style of compute that calculates a temperature. All fixes that compute temperatures define their own compute by default, as described in their documentation. Thus this option allows the user to override the default method for computing T.

The *press* keyword is used to determine how a fix computes pressure. The specified compute ID must have been previously defined by the user via the *compute* command and it must be a style of compute that calculates a pressure. All fixes that compute pressures define their own compute by default, as described in their documentation. Thus this option allows the user to override the default method for computing P.

The *energy* keyword can be used with fixes that support it. *energy yes* adds a contribution to the potential energy of the system. The fix's global and per-atom energy is included in the calculation performed by the *compute pe* or *compute*

pe/atom commands. See the *thermo_style* command for info on how potential energy is output. For fixes that tally a global energy, it can be printed by using the keyword f_ID in the thermo_style custom command, where ID is the fix-ID of the appropriate fix.

Note: You must also specify the *energy yes* setting for a fix if you are using it when performing an *energy minimization* and if you want the energy and forces it produces to be part of the optimization criteria.

The *virial* keyword can be used with fixes that support it. *virial yes* adds a contribution to the virial of the system. The fix's global and per-atom virial is included in the calculation performed by the *compute pressure* or *compute stress/atom* commands. See the *thermo_style* command for info on how pressure is output.

Note: You must specify the *virial yes* setting for a fix if you are doing *box relaxation* and if you want virial contribution of the fix to be part of the relaxation criteria, although this seems unlikely.

Note: This option is only supported by fixes that explicitly say so. For some of these (e.g. the *fix shake* command) the default setting is *virial yes*, for others it is *virial no*.

For fixes that set or modify forces, it may be possible to select at which *r-RESPA* level the fix operates via the *respa* keyword. The RESPA level at which the fix is active can be selected. This is a number ranging from 1 to the number of levels. If the RESPA level is larger than the current maximum, the outermost level will be used, which is also the default setting. This default can be restored using a value of *0* for the RESPA level. The affected fix has to be enabled to support this feature; if not, *fix_modify* will report an error. Active fixes with a custom RESPA level setting are reported with their specified level at the beginning of a r-RESPA run.

The *dynamic/dof* keyword determines whether the number of atoms N in the fix group and their associated degrees of freedom are re-computed each time a temperature is computed. Only fix styles that calculate their own internal temperature use this option. Currently this is only the *fix rigid/nvt/small* and *fix rigid/npt/small* commands for the purpose of thermostatting rigid body translation and rotation. By default, N and their DOF are assumed to be constant. If you are adding atoms or molecules to the system (see the *fix pour*, *fix deposit*, and *fix gcmc* commands) or expect atoms or molecules to be lost (e.g. due to exiting the simulation box or via *fix evaporate*), then this option should be used to insure the temperature is correctly normalized.

Note: Other thermostatting fixes, such as *fix nvt*, do not use the *dynamic/dof* keyword because they use a temperature compute to calculate temperature. See the *compute_modify dynamic/dof* command for a similar way to insure correct temperature normalization for those thermostats.

The *bodyforces* keyword determines whether the forces and torques acting on rigid bodies are computed *early* at the post-force stage of each timestep (right after per-atom forces have been computed and communicated among processors), or *late* at the final-integrate stage of each timestep (after any other fixes have finished their post-force tasks). Only the rigid-body integration fixes use this option, which includes *fix rigid* and *fix rigid/small*, and their variants, and also *fix poems*.

The default is *late*. If there are other fixes that add forces to individual atoms, then the rigid-body constraints will include these forces when time-integrating the rigid bodies. If *early* is specified, then new fixes can be written that use or modify the per-body force and torque, before time-integration of the rigid bodies occurs. Note however this has the side effect, that fixes such as *fix addforce*, *fix setforce*, *fix spring*, which add forces to individual atoms will have no effect on the motion of the rigid bodies if they are specified in the input script after the fix rigid command. LAMMPS will give a warning if that is the case.

15.50.4 Restrictions

none

15.50.5 Related commands

fix, *compute temp*, *compute pressure*, *thermo_style*

15.50.6 Default

The option defaults are temp = ID defined by fix, press = ID defined by fix, energy = no, virial = different for each fix style, respa = 0, bodyforce = late.

15.51 group command

15.51.1 Syntax

```
group ID style args
```

- ID = user-defined name of the group
- style = *delete* or *clear* or *empty* or *region* or *type* or *id* or *molecule* or *variable* or *include* or *subtract* or *union* or *intersect* or *dynamic* or *static*

```
delete = no args
clear = no args
empty = no args
region args = region-ID
type or id or molecule
  args = list of one or more atom types, atom IDs, or molecule IDs
    any entry in list can be a sequence formatted as A:B or A:B:C where
    A = starting index, B = ending index,
    C = increment between indices, 1 if not specified
  args = logical value
    logical = "<" or "<=" or ">" or ">=" or "==" or "!="
    value = an atom type or atom ID or molecule ID (depending on style)
  args = logical value1 value2
    logical = "<>"
    value1,value2 = atom types or atom IDs or molecule IDs (depending on␣
↪style)
variable args = variable-name
include args = molecule
  molecule = add atoms to group with same molecule ID as atoms already in␣
↪group
subtract args = two or more group IDs
union args = one or more group IDs
intersect args = two or more group IDs
dynamic args = parent-ID keyword value ...
  one or more keyword/value pairs may be appended
  keyword = region or var or every
    region value = region-ID
```

```
        var value = name of variable
        property value = name of per-atom property
        every value = N = update group every this many timesteps
    static = no args
```

15.51.2 Examples

```
group edge region regstrip
group water type 3 4
group sub id 10 25 50
group sub id 10 25 50 500:1000
group sub id 100:10000:10
group sub id <= 150
group polyA molecule <> 50 250
group hienergy variable eng
group hienergy include molecule
group boundary subtract all a2 a3
group boundary union lower upper
group boundary intersect upper flow
group boundary delete
group mine dynamic all region myRegion every 100
```

15.51.3 Description

Identify a collection of atoms as belonging to a group. The group ID can then be used in other commands such as *fix*, *compute*, *dump*, or *velocity* to act on those atoms together.

If the group ID already exists, the group command adds the specified atoms to the group.

Note: By default groups are static, meaning the atoms are permanently assigned to the group. For example, if the *region* style is used to assign atoms to a group, the atoms will remain in the group even if they later move out of the region. As explained below, the *dynamic* style can be used to make a group dynamic so that a periodic determination is made as to which atoms are in the group. Since many LAMMPS commands operate on groups of atoms, you should think carefully about whether making a group dynamic makes sense for your model.

A group with the ID *all* is predefined. All atoms belong to this group. This group cannot be deleted, or made dynamic.

The *delete* style removes the named group and un-assigns all atoms that were assigned to that group. Since there is a restriction (see below) that no more than 32 groups can be defined at any time, the *delete* style allows you to remove groups that are no longer needed, so that more can be specified. You cannot delete a group if it has been used to define a current *fix* or *compute* or *dump*.

The *clear* style un-assigns all atoms that were assigned to that group. This may be dangerous to do during a simulation run, e.g. using the *run every* command if a fix or compute or other operation expects the atoms in the group to remain constant, but LAMMPS does not check for this.

The *empty* style creates an empty group, which is useful for commands like *fix gcmc* or with complex scripts that add atoms to a group.

The *region* style puts all atoms in the region volume into the group. Note that this is a static one-time assignment. The atoms remain assigned (or not assigned) to the group even in they later move out of the region volume.

The *type*, *id*, and *molecule* styles put all atoms with the specified atom types, atom IDs, or molecule IDs into the group. These 3 styles can use arguments specified in one of two formats.

The first format is a list of values (types or IDs). For example, the 2nd command in the examples above puts all atoms of type 3 or 4 into the group named *water*. Each entry in the list can be a colon-separated sequence A:B or A:B:C, as in two of the examples above. A "sequence" generates a sequence of values (types or IDs), with an optional increment. The first example with 500:1000 has the default increment of 1 and would add all atom IDs from 500 to 1000 (inclusive) to the group sub, along with 10,25,50 since they also appear in the list of values. The second example with 100:10000:10 uses an increment of 10 and would thus would add atoms IDs 100,110,120, . . . 9990,10000 to the group sub.

The second format is a *logical* followed by one or two values (type or ID). The 7 valid logicals are listed above. All the logicals except <> take a single argument. The 3rd example above adds all atoms with IDs from 1 to 150 to the group named *sub*. The logical <> means "between" and takes 2 arguments. The 4th example above adds all atoms belonging to molecules with IDs from 50 to 250 (inclusive) to the group named polyA.

The *variable* style evaluates a variable to determine which atoms to add to the group. It must be an *atom-style variable* previously defined in the input script. If the variable evaluates to a non-zero value for a particular atom, then that atom is added to the specified group.

Atom-style variables can specify formulas that include thermodynamic quantities, per-atom values such as atom coordinates, or per-atom quantities calculated by computes, fixes, or other variables. They can also include Boolean logic where 2 numeric values are compared to yield a 1 or 0 (effectively a true or false). Thus using the *variable* style, is a general way to flag specific atoms to include or exclude from a group.

For example, these lines define a variable "eatom" that calculates the potential energy of each atom and includes it in the group if its potential energy is above the threshold value -3.0.

```
compute         1 all pe/atom
compute         2 all reduce sum c_1
thermo_style    custom step temp pe c_2
run             0

variable        eatom atom "c_1 > -3.0"
group           hienergy variable eatom
```

Note that these lines

```
compute         2 all reduce sum c_1
thermo_style    custom step temp pe c_2
run             0
```

are necessary to insure that the "eatom" variable is current when the group command invokes it. Because the eatom variable computes the per-atom energy via the pe/atom compute, it will only be current if a run has been performed which evaluated pairwise energies, and the pe/atom compute was actually invoked during the run. Printing the thermodynamic info for compute 2 insures that this is the case, since it sums the pe/atom compute values (in the reduce compute) to output them to the screen. See the "Variable Accuracy" section of the *variable* doc page for more details on insuring that variables are current when they are evaluated between runs.

The *include* style with its arg *molecule* adds atoms to a group that have the same molecule ID as atoms already in the group. The molecule ID = 0 is ignored in this operation, since it is assumed to flag isolated atoms that are not part of molecules. An example of where this operation is useful is if the *region* style has been used previously to add atoms to a group that are within a geometric region. If molecules straddle the region boundary, then atoms outside the region that are part of molecules with atoms inside the region will not be in the group. Using the group command a 2nd time with *include molecule* will add those atoms that are outside the region to the group.

Note: The *include molecule* operation is relatively expensive in a parallel sense. This is because it requires communication of relevant molecule IDs between all the processors and each processor to loop over its atoms once per processor, to compare its atoms to the list of molecule IDs from every other processor. Hence it scales as N, rather

than N/P as most of the group operations do, where N is the number of atoms, and P is the number of processors.

The *subtract* style takes a list of two or more existing group names as arguments. All atoms that belong to the 1st group, but not to any of the other groups are added to the specified group.

The *union* style takes a list of one or more existing group names as arguments. All atoms that belong to any of the listed groups are added to the specified group.

The *intersect* style takes a list of two or more existing group names as arguments. Atoms that belong to every one of the listed groups are added to the specified group.

The *dynamic* style flags an existing or new group as dynamic. This means atoms will be (re)assigned to the group periodically as a simulation runs. This is in contrast to static groups where atoms are permanently assigned to the group. The way the assignment occurs is as follows. Only atoms in the group specified as the parent group via the parent-ID are assigned to the dynamic group before the following conditions are applied. If the *region* keyword is used, atoms not in the specified region are removed from the dynamic group. If the *var* keyword is used, the variable name must be an atom-style or atomfile-style variable. The variable is evaluated and atoms whose per-atom values are 0.0, are removed from the dynamic group. If the *property* keyword is used, the per-atom property name must be a previously defined per-atom property. The per-atom property is evaluated and atoms whose values are 0.0 are removed from the dynamic group.

The assignment of atoms to a dynamic group is done at the beginning of each run and on every timestep that is a multiple of *N*, which is the argument for the *every* keyword (N = 1 is the default). For an energy minimization, via the *minimize* command, an assignment is made at the beginning of the minimization, but not during the iterations of the minimizer.

The point in the timestep at which atoms are assigned to a dynamic group is after the initial stage of velocity Verlet time integration has been performed, and before neighbor lists or forces are computed. This is the point in the timestep where atom positions have just changed due to the time integration, so the region criterion should be accurate, if applied.

Note: If the *region* keyword is used to determine what atoms are in the dynamic group, atoms can move outside of the simulation box between reneighboring events. Thus if you want to include all atoms on the left side of the simulation box, you probably want to set the left boundary of the region to be outside the simulation box by some reasonable amount (e.g. up to the cutoff of the potential), else they may be excluded from the dynamic region.

Here is an example of using a dynamic group to shrink the set of atoms being integrated by using a spherical region with a variable radius (shrinking from 18 to 5 over the course of the run). This could be used to model a quench of the system, freezing atoms outside the shrinking sphere, then converting the remaining atoms to a static group and running further.

```
variable        nsteps equal 5000
variable        rad equal 18-(step/v_nsteps)*(18-5)
region          ss sphere 20 20 0 v_rad
group           mobile dynamic all region ss
fix             1 mobile nve
run             ${nsteps}
group           mobile static
run             ${nsteps}
```

Note: All fixes and computes take a group ID as an argument, but they do not all allow for use of a dynamic group. If you get an error message that this is not allowed, but feel that it should be for the fix or compute in question, then please post your reasoning to the LAMMPS mail list and we can change it.

The *static* style removes the setting for a dynamic group, converting it to a static group (the default). The atoms in the static group are those currently in the dynamic group.

15.51.4 Restrictions

There can be no more than 32 groups defined at one time, including "all".

The parent group of a dynamic group cannot itself be a dynamic group.

15.51.5 Related commands

dump, *fix*, *region*, *velocity*

15.51.6 Default

All atoms belong to the "all" group.

15.52 group2ndx command

15.53 ndx2group command

15.53.1 Syntax

```
group2ndx file group-ID ...
ndx2group file group-ID ...
```

- file = name of index file to write out or read in
- zero or more group IDs may be appended

15.53.2 Examples

```
group2ndx allindex.ndx
group2ndx someindex.ndx upper lower mobile
ndx2group someindex.ndx
ndx2group someindex.ndx mobile
```

15.53.3 Description

Write or read a Gromacs style index file in text format that associates atom IDs with the corresponding group definitions. This index file can be used with in combination with Gromacs analysis tools or to import group definitions into the *fix colvars* input file. It can also be used to save and restore group definitions for static groups.

The *group2ndx* command will write group definitions to an index file. Without specifying any group IDs, all groups will be written to the index file. When specifying group IDs, only those groups will be written to the index file. In order to follow the Gromacs conventions, the group *all* will be renamed to *System* in the index file.

The *ndx2group* command will create of update group definitions from those stored in an index file. Without specifying any group IDs, all groups except *System* will be read from the index file and the corresponding groups recreated. If a group of the same name already exists, it will be completely reset. When specifying group IDs, those groups, if present, will be read from the index file and restored.

15.53.4 Restrictions

This command requires that atoms have atom IDs, since this is the information that is written to the index file.

These commands are part of the USER-COLVARS package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

15.53.5 Related commands

group, *dump*, *fix colvars*

Default: none

15.54 hyper command

15.54.1 Syntax

```
hyper N Nevent fix-ID compute-ID keyword values ...
```

- N = # of timesteps to run
- Nevent = check for events every this many steps
- fix-ID = ID of a fix that applies a global or local bias potential, can be NULL
- compute-ID = ID of a compute that identifies when an event has occurred
- zero or more keyword/value pairs may be appended
- keyword = *min* or *dump* or *rebond*

```
min values = etol ftol maxiter maxeval
  etol = stopping tolerance for energy, used in quenching
  ftol = stopping tolerance for force, used in quenching
  maxiter = max iterations of minimize, used in quenching
  maxeval = max number of force/energy evaluations, used in quenching
dump value = dump-ID
  dump-ID = ID of dump to trigger whenever an event takes place
```

```
rebond value = Nrebond
  Nrebond = frequency at which to reset bonds, even if no event has␣
↪occurred
```

15.54.2 Examples

```
compute event all event/displace 1.0
fix HG mobile hyper/global 3.0 0.3 0.4 800.0
hyper 5000 100 HG event min 1.0e-6 1.0e-6 100 100 dump 1 dump 5
```

15.54.3 Description

Run a bond-boost hyperdynamics (HD) simulation where time is accelerated by application of a bias potential to one or more pairs of nearby atoms in the system. This command can be used to run both global and local hyperdynamics. In global HD a single bond within the system is biased on each timestep. In local HD multiple bonds (separated by a sufficient distance) can be biased simultaneously at each timestep. In the bond-boost hyperdynamics context, a "bond" is not a covalent bond between a pair of atoms in a molecule. Rather it is simply a pair of nearby atoms as discussed below.

Both global and local HD are described in *(Voter2013)* by Art Voter and collaborators. Similar to parallel replica dynamics (PRD), global and local HD are methods for performing accelerated dynamics that are suitable for infrequent-event systems that obey first-order kinetics. A good overview of accelerated dynamics methods for such systems in given in *(Voter2002)* from the same group. To quote from the review paper: "The dynamical evolution is characterized by vibrational excursions within a potential basin, punctuated by occasional transitions between basins." The transition probability is characterized by p(t) = k*exp(-kt) where k is the rate constant. Running multiple replicas gives an effective enhancement in the timescale spanned by the multiple simulations, while waiting for an event to occur.

Both HD and PRD produce a time-accurate trajectory that effectively extends the timescale over which a system can be simulated, but they do it differently. HD uses a single replica of the system and accelerates time by biasing the interaction potential in a manner such that each timestep is effectively longer. PRD creates Nr replicas of the system and runs dynamics on each independently with a normal unbiased potential until an event occurs in one of the replicas. The time between events is reduced by a factor of Nr replicas. For both methods, per CPU second, more physical time elapses and more events occur. See the *prd* doc page for more info about PRD.

An HD run has several stages, which are repeated each time an event occurs, as explained below. The logic for an HD run is as follows:

```
quench
create initial list of bonds

while (time remains):
  run dynamics for Nevent steps
  quench
  check for an event
  if event occurred: reset list of bonds
  restore pre-quench state
```

The list of bonds is the list of atom pairs of atoms that are within a short cutoff distance of each other after the system energy is minimized (quenched). This list is created and reset by a *fix hyper/global* or *fix hyper/local* command specified as *fix-ID*. At every dynamics timestep, the same fix selects one of more bonds to apply a bias potential to.

Note: The style of fix associated with the specified *fix-ID* determines whether you are running the global versus local hyperdynamics algorithm.

Dynamics (with the bias potential) is run continuously, stopping every *Nevent* steps to check if a transition event has occurred. The specified *N* for total steps must be a multiple of *Nevent*. check is performed by quenching the system and comparing the resulting atom coordinates to the coordinates from the previous basin.

A quench is an energy minimization and is performed by whichever algorithm has been defined by the *min_style* command. Minimization parameters may be set via the *min_modify* command and by the *min* keyword of the hyper command. The latter are the settings that would be used with the *minimize* command. Note that typically, you do not need to perform a highly-converged minimization to detect a transition event, though you may need to in order to prevent a set of atoms in the system from relaxing to a saddle point.

The event check is performed by a compute with the specified *compute-ID*. Currently there is only one compute that works with the hyper command, which is the *compute event/displace* command. Other event-checking computes may be added. *Compute event/displace* checks whether any atom in the compute group has moved further than a specified threshold distance. If so, an event has occurred.

If this happens, the list of bonds is reset, since some bond pairs are likely now too far apart, and new pairs are likely close enough to be considered a bond. The pre-quenched state of the system (coordinates and velocities) is restored, and dynamics continue.

At the end of the hyper run, a variety of statistics are output to the screen and logfile. These include info relevant to both global and local hyperdynamics, such as the number of events and the elapsed hyper time (accelerated time), And it includes info specific to one or the other, depending on which style of fix was specified by *fix-ID*.

The optional keywords operate as follows.

As explained above, the *min* keyword can be used to specify parameters for the quench. Their meaning is the same as for the *minimize* command

The *dump* keyword can be used to trigger a specific dump command with the specified *dump-ID* to output a snapshot each time an event is detected. It can be specified multiple times with different *dump-ID* values, as in the example above. These snapshots will be for the quenched state of the system on a timestep that is a multiple of *Nevent*, i.e. a timestep after the event has occurred. Note that any dump command in the input script will also output snapshots at whatever timestep interval it defines via its *N* argument; see the *dump* command for details. This means if you only want a particular dump to output snapshots when events are detected, you should specify its *N* as a value larger than the length of the hyperdynamics run.

As in the code logic above, the bond list is normally only reset when an event occurs. The *rebond* keyword will force a reset of the bond list every *Nrebond* steps, even if an event has not occurred. *Nrebond* must be a multiple of *Nevent*. This can be useful to check if more frequent resets alter event statistics, perhaps because the parameters chosen for defining what is a bond and what is an event are producing bad dynamics in the presence of the bias potential.

15.54.4 Restrictions

This command can only be used if LAMMPS was built with the REPLICA package. See the *Build package* doc page for more info.

15.54.5 Related commands

fix hyper/global, *fix hyper/local*, *compute event/displace*, *prd*

15.54.6 Default

The option defaults are min = 0.1 0.1 40 50 and time = steps.

(Voter2013) S. Y. Kim, D. Perez, A. F. Voter, J Chem Phys, 139, 144110 (2013).

(Voter2002) Voter, Montalenti, Germann, Annual Review of Materials Research 32, 321 (2002).

15.55 if command

15.55.1 Syntax

```
if boolean then t1 t2 ... elif boolean f1 f2 ... elif boolean f1 f2 ... else e1 e2 ...
```

- boolean = a Boolean expression evaluated as TRUE or FALSE (see below)
- then = required word
- t1,t2,...,tN = one or more LAMMPS commands to execute if condition is met, each enclosed in quotes
- elif = optional word, can appear multiple times
- f1,f2,...,fN = one or more LAMMPS commands to execute if elif condition is met, each enclosed in quotes (optional arguments)
- else = optional argument
- e1,e2,...,eN = one or more LAMMPS commands to execute if no condition is met, each enclosed in quotes (optional arguments)

15.55.2 Examples

```
if "${steps} > 1000" then quit
if "${myString} == a10" then quit
if "$x <= $y" then "print X is smaller = $x" else "print Y is smaller = $y"
if "(${eng} > 0.0) || ($n < 1000)" then &
  "timestep 0.005" &
elif $n<10000 &
  "timestep 0.01" &
else &
  "timestep 0.02" &
  "print 'Max step reached'"
if "${eng} > ${eng_previous}" then "jump file1" else "jump file2"
```

15.55.3 Description

This command provides an if-then-else capability within an input script. A Boolean expression is evaluated and the result is TRUE or FALSE. Note that as in the examples above, the expression can contain variables, as defined by the *variable* command, which will be evaluated as part of the expression. Thus a user-defined formula that reflects the current state of the simulation can be used to issue one or more new commands.

If the result of the Boolean expression is TRUE, then one or more commands (t1, t2, ..., tN) are executed. If it is FALSE, then Boolean expressions associated with successive elif keywords are evaluated until one is found to be true, in which case its commands (f1, f2, ..., fN) are executed. If no Boolean expression is TRUE, then the commands associated with the else keyword, namely (e1, e2, ..., eN), are executed. The elif and else keywords and their associated commands are optional. If they aren't specified and the initial Boolean expression is FALSE, then no commands are executed.

The syntax for Boolean expressions is described below.

Each command (t1, f1, e1, etc) can be any valid LAMMPS input script command. If the command is more than one word, it must enclosed in quotes, so it will be treated as a single argument, as in the examples above.

Note: If a command itself requires a quoted argument (e.g. a *print* command), then double and single quotes can be used and nested in the usual manner, as in the examples above and below. The *Commands parse* doc page has more details on using quotes in arguments. Only one of level of nesting is allowed, but that should be sufficient for most use cases.

Note that by using the line continuation character "&", the if command can be spread across many lines, though it is still a single command:

```
if "$a < $b" then &
  "print 'Minimum value = $a'" &
  "run 1000" &
else &
  'print "Minimum value = $b"' &
  "minimize 0.001 0.001 1000 10000"
```

Note that if one of the commands to execute is *quit*, as in the first example above, then executing the command will cause LAMMPS to halt.

Note that by jumping to a label in the same input script, the if command can be used to break out of a loop. See the *variable delete* command for info on how to delete the associated loop variable, so that it can be re-used later in the input script.

Here is an example of a loop which checks every 1000 steps if the system temperature has reached a certain value, and if so, breaks out of the loop to finish the run. Note that any variable could be checked, so long as it is current on the timestep when the run completes. As explained on the *variable* doc page, this can be insured by including the variable in thermodynamic output.

```
variable myTemp equal temp
label loop
variable a loop 1000
run 1000
if "${myTemp} < 300.0" then "jump SELF break"
next a
jump SELF loop
label break
print "ALL DONE"
```

Here is an example of a double loop which uses the if and *jump* commands to break out of the inner loop when a condition is met, then continues iterating through the outer loop.

```
label       loopa
variable    a loop 5
  label     loopb
  variable  b loop 5
  print     "A,B = $a,$b"
  run       10000
  if        "$b > 2" then "jump SELF break"
  next      b
  jump      in.script loopb
label       break
variable    b delete
next        a
jump        SELF loopa
```

The Boolean expressions for the if and elif keywords have a C-like syntax. Note that each expression is a single argument within the if command. Thus if you want to include spaces in the expression for clarity, you must enclose the entire expression in quotes.

An expression is built out of numbers (which start with a digit or period or minus sign) or strings (which start with a letter and can contain alphanumeric characters or underscores):

```
0.2, 100, 1.0e20, -15.4, etc
InP, myString, a123, ab_23_cd, etc
```

and Boolean operators:

```
A == B, A != B, A < B, A <= B, A > B, A >= B, A && B, A || B, A |^ B, !A
```

Each A and B is a number or string or a variable reference like $a or ${abc}, or A or B can be another Boolean expression.

If a variable is used it can produce a number when evaluated, like an *equal-style variable*. Or it can produce a string, like an *index-style variable*. For an individual Boolean operator, A and B must both be numbers or must both be strings. You cannot compare a number to a string.

Expressions are evaluated left to right and have the usual C-style precedence: the unary logical NOT operator "!" has the highest precedence, the 4 relational operators "<", "<=", ">", and ">=" are next; the two remaining relational operators "==" and "!=" are next; then the logical AND operator "&&"; and finally the logical OR operator "||" and logical XOR (exclusive or) operator "|^" have the lowest precedence. Parenthesis can be used to group one or more portions of an expression and/or enforce a different order of evaluation than what would occur with the default precedence.

When the 6 relational operators (first 6 in list above) compare 2 numbers, they return either a 1.0 or 0.0 depending on whether the relationship between A and B is TRUE or FALSE. When the 6 relational operators compare 2 strings, they also return a 1.0 or 0.0 for TRUE or FALSE, but the comparison is done by the C function strcmp().

When the 3 logical operators (last 3 in list above) compare 2 numbers, they also return either a 1.0 or 0.0 depending on whether the relationship between A and B is TRUE or FALSE (or just A). The logical AND operator will return 1.0 if both its arguments are non-zero, else it returns 0.0. The logical OR operator will return 1.0 if either of its arguments is non-zero, else it returns 0.0. The logical XOR operator will return 1.0 if one of its arguments is zero and the other non-zero, else it returns 0.0. The logical NOT operator returns 1.0 if its argument is 0.0, else it returns 0.0. The 3 logical operators can only be used to operate on numbers, not on strings.

The overall Boolean expression produces a TRUE result if the result is non-zero. If the result is zero, the expression result is FALSE.

15.55.4 Restrictions

none

15.55.5 Related commands

variable, *print*

Default: none

15.56 improper_coeff command

15.56.1 Syntax

```
improper_coeff N args
```

- N = improper type (see asterisk form below)
- args = coefficients for one or more improper types

15.56.2 Examples

```
improper_coeff 1 300.0 0.0
improper_coeff * 80.2 -1 2
improper_coeff *4 80.2 -1 2
```

15.56.3 Description

Specify the improper force field coefficients for one or more improper types. The number and meaning of the coefficients depends on the improper style. Improper coefficients can also be set in the data file read by the *read_data* command or in a restart file.

N can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to set the coefficients for multiple improper types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of improper types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

Note that using an improper_coeff command can override a previous setting for the same improper type. For example, these commands set the coeffs for all improper types, then overwrite the coeffs for just improper type 2:

```
improper_coeff * 300.0 0.0
improper_coeff 2 50.0 0.0
```

A line in a data file that specifies improper coefficients uses the exact same format as the arguments of the improper_coeff command in an input script, except that wild-card asterisks should not be used since coefficients for all N types must be listed in the file. For example, under the "Improper Coeffs" section of a data file, the line that corresponds to the 1st example above would be listed as

```
1 300.0 0.0
```

The *improper_style class2* is an exception to this rule, in that an additional argument is used in the input script to allow specification of the cross-term coefficients. See its doc page for details.

The list of all improper styles defined in LAMMPS is given on the *improper_style* doc page. They are also listed in more compact form on the *Commands improper* doc page.

On either of those pages, click on the style to display the formula it computes and its coefficients as specified by the associated improper_coeff command.

15.56.4 Restrictions

This command must come after the simulation box is defined by a *read_data*, *read_restart*, or *create_box* command.

An improper style must be defined before any improper coefficients are set, either in the input script or in a data file.

15.56.5 Related commands

improper_style

Default: none

15.57 improper_style command

15.57.1 Syntax

```
improper_style style
```

- style = *none* or *hybrid* or *class2* or *cvff* or *harmonic*

15.57.2 Examples

```
improper_style harmonic
improper_style cvff
improper_style hybrid cvff harmonic
```

15.57.3 Description

Set the formula(s) LAMMPS uses to compute improper interactions between quadruplets of atoms, which remain in force for the duration of the simulation. The list of improper quadruplets is read in by a *read_data* or *read_restart* command from a data or restart file. Note that the ordering of the 4 atoms in an improper quadruplet determines the definition of the improper angle used in the formula for each style. See the doc pages of individual styles for details.

Hybrid models where impropers are computed using different improper potentials can be setup using the *hybrid* improper style.

The coefficients associated with an improper style can be specified in a data or restart file or via the *improper_coeff* command.

All improper potentials store their coefficient data in binary restart files which means improper_style and *improper_coeff* commands do not need to be re-specified in an input script that restarts a simulation. See the *read_restart* command for details on how to do this. The one exception is that improper_style *hybrid* only stores the list of sub-styles in the restart file; improper coefficients need to be re-specified.

Note: When both an improper and pair style is defined, the *special_bonds* command often needs to be used to turn off (or weight) the pairwise interaction that would otherwise exist between a group of 4 bonded atoms.

Here is an alphabetic list of improper styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated *improper_coeff* command.

Click on the style to display the formula it computes, any additional arguments specified in the improper_style command, and coefficients specified by the associated *improper_coeff* command.

There are also additional accelerated pair styles included in the LAMMPS distribution for faster performance on CPUs, GPUs, and KNLs. The individual style names on the *Commands improper* doc page are followed by one or more of (g,i,k,o,t) to indicate which accelerated styles exist.

- *none* - turn off improper interactions
- *zero* - topology but no interactions
- *hybrid* - define multiple styles of improper interactions
- *class2* - COMPASS (class 2) improper
- *cossq* - improper with a cosine squared term
- *cvff* - CVFF improper
- *distance* - improper based on distance between atom planes
- *distharm* - improper that is harmonic in the out-of-plane distance
- *fourier* - improper with multiple cosine terms
- *harmonic* - harmonic improper
- *inversion/harmonic* - harmonic improper with Wilson-Decius out-of-plane definition
- *ring* - improper which prevents planar conformations
- *umbrella* - DREIDING improper

sqdistharm - improper that is harmonic in the square of the out-of-plane distance

---

15.57.4 Restrictions

Improper styles can only be set for atom_style choices that allow impropers to be defined.

Most improper styles are part of the MOLECULE package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info. The doc pages for individual improper potentials tell if it is part of a package.

15.57.5 Related commands

improper_coeff

15.57.6 Default

```
improper_style none
```

15.58 include command

15.58.1 Syntax

```
include file
```

- file = filename of new input script to switch to

15.58.2 Examples

```
include newfile
include in.run2
```

15.58.3 Description

This command opens a new input script file and begins reading LAMMPS commands from that file. When the new file is finished, the original file is returned to. Include files can be nested as deeply as desired. If input script A includes script B, and B includes A, then LAMMPS could run for a long time.

If the filename is a variable (see the *variable* command), different processor partitions can run different input scripts.

15.58.4 Restrictions

none

15.58.5 Related commands

variable, *jump*

Default: none

15.59 info command

15.59.1 Syntax

```
info args
```

- args = one or more of the following keywords: *out*, *all*, *system*, *memory*, *communication*, *computes*, *dumps*, *fixes*, *groups*, *regions*, *variables*, *coeffs*, *styles*, *time*, or *configuration*
- *out* values = *screen*, *log*, *append* filename, *overwrite* filename
- *styles* values = *all*, *angle*, *atom*, *bond*, *compute*, *command*, *dump*, *dihedral*, *fix*, *improper*, *integrate*, *kspace*, *minimize*, *pair*, *region*

15.59.2 Examples

```
info system
info groups computes variables
info all out log
info all out append info.txt
info styles all
info styles atom
```

15.59.3 Description

Print out information about the current internal state of the running LAMMPS process. This can be helpful when debugging or validating complex input scripts. Several output categories are available and one or more output category may be requested.

The *out* flag controls where the output is sent. It can only be sent to one target. By default this is the screen, if it is active. The *log* argument selects the log file instead. With the *append* and *overwrite* option, followed by a filename, the output is written to that file, which is either appended to or overwritten, respectively.

The *all* flag activates printing all categories listed below.

The *configuration* category prints some information about the LAMMPS version as well as architecture and OS it is run on.

The *memory* category prints some information about the current memory allocation of MPI rank 0 (this the amount of dynamically allocated memory reported by LAMMPS classes). Where supported, also some OS specific information about the size of the reserved memory pool size (this is where malloc() and the new operator request memory from) and the maximum resident set size is reported (this is the maximum amount of physical memory occupied so far).

The *system* category prints a general system overview listing. This includes the unit style, atom style, number of atoms, bonds, angles, dihedrals, and impropers and the number of the respective types, box dimensions and properties, force computing styles and more.

The *communication* category prints a variety of information about communication and parallelization: the MPI library version level, the number of MPI ranks and OpenMP threads, the communication style and layout, the processor grid dimensions, ghost atom communication mode, cutoff, and related settings.

The *computes* category prints a list of all currently defined computes, their IDs and styles and groups they operate on.

The *dumps* category prints a list of all currently active dumps, their IDs, styles, filenames, groups, and dump frequencies.

The *fixes* category prints a list of all currently defined fixes, their IDs and styles and groups they operate on.

The *groups* category prints a list of all currently defined groups.

The *regions* category prints a list of all currently defined regions, their IDs and styles and whether "inside" or "outside" atoms are selected.

The *variables* category prints a list of all currently defined variables, their names, styles, definition and last computed value, if available.

The *coeffs* category prints a list for each defined force style (pair, bond, angle, dihedral, improper) indicating which of the corresponding coefficients have been set. This can be very helpful to debug error messages like "All pair coeffs are not set".

The *styles* category prints the list of styles available in the current LAMMPS binary. It supports one of the following options to control which category of styles is printed out:

- all
- angle
- atom
- bond
- compute
- command
- dump
- dihedral
- fix
- improper
- integrate
- kspace
- minimize
- pair
- region

The *time* category prints the accumulated CPU and wall time for the process that writes output (usually MPI rank 0).

15.59.4 Restrictions

none

15.59.5 Related commands

print

15.59.6 Default

The *out* option has the default *screen*.

The *styles* option has the default *all*.

15.60 jump command

15.60.1 Syntax

```
jump file label
```

- file = filename of new input script to switch to
- label = optional label within file to jump to

15.60.2 Examples

```
jump newfile
jump in.run2 runloop
jump SELF runloop
```

15.60.3 Description

This command closes the current input script file, opens the file with the specified name, and begins reading LAMMPS commands from that file. Unlike the *include* command, the original file is not returned to, although by using multiple jump commands it is possible to chain from file to file or back to the original file.

If the word "SELF" is used for the filename, then the current input script is re-opened and read again.

Note: The SELF option is not guaranteed to work when the current input script is being read through stdin (standard input), e.g.

```
lmp_g++ < in.script
```

since the SELF option invokes the C-library rewind() call, which may not be supported for stdin on some systems or by some MPI implementations. This can be worked around by using the *-in command-line switch*, e.g.

```
lmp_g++ -in in.script
```

or by using the *-var command-line switch* to pass the script name as a variable to the input script. In the latter case, a *variable* called "fname" could be used in place of SELF, e.g.

```
lmp_g++ -var fname in.script < in.script
```

The 2nd argument to the jump command is optional. If specified, it is treated as a label and the new file is scanned (without executing commands) until the label is found, and commands are executed from that point forward. This can be used to loop over a portion of the input script, as in this example. These commands perform 10 runs, each of 10000 steps, and create 10 dump files named file.1, file.2, etc. The *next* command is used to exit the loop after 10 iterations. When the "a" variable has been incremented for the tenth time, it will cause the next jump command to be skipped.

```
variable a loop 10
label loop
dump 1 all atom 100 file.$a
run 10000
undump 1
next a
jump in.lj loop
```

If the jump *file* argument is a variable, the jump command can be used to cause different processor partitions to run different input scripts. In this example, LAMMPS is run on 40 processors, with 4 partitions of 10 procs each. An in.file containing the example variable and jump command will cause each partition to run a different simulation.

```
mpirun -np 40 lmp_ibm -partition 4x10 -in in.file

variable f world script.1 script.2 script.3 script.4
jump $f
```

Here is an example of a loop which checks every 1000 steps if the system temperature has reached a certain value, and if so, breaks out of the loop to finish the run. Note that any variable could be checked, so long as it is current on the timestep when the run completes. As explained on the *variable* doc page, this can be insured by including the variable in thermodynamic output.

```
variable myTemp equal temp
label loop
variable a loop 1000
run 1000
if "${myTemp} < 300.0" then "jump SELF break"
next a
jump SELF loop
label break
print "ALL DONE"
```

Here is an example of a double loop which uses the if and *jump* commands to break out of the inner loop when a condition is met, then continues iterating through the outer loop.

```
label       loopa
variable    a loop 5
  label     loopb
  variable  b loop 5
  print     "A,B = $a,$b"
  run       10000
  if        "$b > 2" then "jump SELF break"
  next      b
  jump      in.script loopb
label       break
variable    b delete
```

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```
next        a
jump        SELF loopa
```

15.60.4 Restrictions

If you jump to a file and it does not contain the specified label, LAMMPS will come to the end of the file and exit.

15.60.5 Related commands

variable, *include*, *label*, *next*

Default: none

15.61 kim_init command

15.62 kim_interactions command

15.63 kim_query command

15.64 kim_param command

15.64.1 Syntax

```
kim_init model user_units unitarg
kim_interactions typeargs
kim_query variable formatarg query_function queryargs
kim_param get param_name index_range variables formatarg
kim_param set param_name index_range values
```

- model = name of the KIM interatomic model (the KIM ID for models archived in OpenKIM)
- user_units = the LAMMPS *units* style assumed in the LAMMPS input script
- unitarg = *unit_conversion_mode* (optional)
- typeargs = atom type to species mapping (one entry per atom type) or *fixed_types* for models with a preset fixed mapping
- variable(s) = single name or list of names of (string style) LAMMPS variable(s) where a query result or parameter get result is stored. Variables that do not exist will be created by the command.
- formatarg = *list, split, or explicit* (optional):

```
list = returns a single string with a list of space separated values
       (e.g. "1.0 2.0 3.0"), which is placed in a LAMMPS variable as
       defined by the variable argument. [default for kim_query]
split = returns the values separately in new variables with names based
       on the prefix specified in variable and a number appended to
       indicate which element in the list of values is in the variable.
explicit = returns the values separately in one more more variable names
```

```
        provided as arguments that preceed formatarg. [default for kim_
↪param]
```

- query_function = name of the OpenKIM web API query function to be used
- queryargs = a series of *keyword*=*value* pairs that represent the web query; supported keywords depend on the query function
- param_name = name of a KIM portable model parameter
- index_range = KIM portable model parameter index range (an integer for a single element, or pair of integers separated by a colon for a range of elements)
- values = new value(s) to replace the current value(s) of a KIM portable model parameter

15.64.2 Examples

```
kim_init SW_StillingerWeber_1985_Si__MO_405512056662_005 metal
kim_interactions Si
kim_init Sim_LAMMPS_ReaxFF_StrachanVanDuinChakraborty_2003_CHNO__SM_107643900657_000␣
↪real
kim_init Sim_LAMMPS_ReaxFF_StrachanVanDuinChakraborty_2003_CHNO__SM_107643900657_000␣
↪metal unit_conversion_mode
kim_interactions C H O
kim_init Sim_LAMMPS_IFF_PCFF_HeinzMishraLinEmami_2015Ver1v5_
↪FccmetalsMineralsSolventsPolymers__SM_039297821658_000 real
kim_interactions fixed_types
kim_query a0 get_lattice_constant_cubic crystal=["fcc"] species=["Al"] units=[
↪"angstrom"]
kim_param get gamma 1 varGamma
kim_param set gamma 1 3.0
```

15.64.3 Description

The set of *kim_commands* provide a high-level wrapper around the Open Knowledgebase of Interatomic Models (OpenKIM) repository of interatomic models (IMs) (potentials and force fields), so that they can be used by LAMMPS scripts. These commands do not implement any computations directly, but rather generate LAMMPS input commands based on the information retrieved from the OpenKIM repository to initialize and activate OpenKIM IMs and query their predictions for use in the LAMMPS script. All LAMMPS input commands generated and executed by *kim_commands* are echoed to the LAMMPS log file.

Benefits of Using OpenKIM IMs

Employing OpenKIM IMs provides LAMMPS users with multiple benefits:

Reliability

- All content archived in OpenKIM is reviewed by the KIM Editor for quality.
- IMs in OpenKIM are archived with full provenance control. Each is associated with a maintainer responsible for the integrity of the content. All changes are tracked and recorded.
- IMs in OpenKIM are exhaustively tested using KIM Tests that compute a host of material properties, and KIM Verification Checks that provide the user with information on various aspects of the IM behavior and coding correctness. This information is displayed on the IM's page accessible through the OpenKIM browse interface.

Reproducibility

- Each IM in OpenKIM is issued a unique identifier (KIM ID), which includes a version number (last three digits). Any changes that can result in different numerical values lead to a version increment in the KIM ID. This makes it possible to reproduce simulations since the specific version of a specific IM used can be retrieved using its KIM ID.
- OpenKIM is a member organization of DataCite and issues digital object identifiers (DOIs) to all IMs archived in OpenKIM. This makes it possible to cite the IM code used in a simulation in a publications to give credit to the developers and further facilitate reproducibility.

Convenience

- IMs in OpenKIM are distributed in binary form along with LAMMPS and can be used in a LAMMPS input script simply by providing their KIM ID in the *kim_init* command documented on this page.
- The *kim_query* web query tool provides the ability to use the predictions of IMs for supported material properties (computed via KIM Tests) as part of a LAMMPS input script setup and analysis.
- Support is provided for unit conversion between the *unit style* used in the LAMMPS input script and the units required by the OpenKIM IM. This makes it possible to use a single input script with IMs using different units without change and minimizes the likelihood of errors due to incompatible units.

Types of IMs in OpenKIM

There are two types of IMs archived in OpenKIM:

1. The first type is called a *KIM Portable Model* (PM). A KIM PM is an independent computer implementation of an IM written in one of the languages supported by KIM (C, C++, Fortran) that conforms to the KIM Application Programming Interface (KIM API) Portable Model Interface (PMI) standard. A KIM PM will work seamlessly with any simulation code that supports the KIM API/PMI standard (including LAMMPS; see complete list of supported codes).
2. The second type is called a *KIM Simulator Model* (SM). A KIM SM is an IM that is implemented natively within a simulation code (*simulator*) that supports the KIM API Simulator Model Interface (SMI); in this case LAMMPS. A separate SM package is archived in OpenKIM for each parameterization of the IM, which includes all of the necessary parameter files, LAMMPS commands, and metadata (supported species, units, etc.) needed to run the IM in LAMMPS.

With these two IM types, OpenKIM can archive and test almost all IMs that can be used by LAMMPS. (It is easy to contribute new IMs to OpenKIM, see the upload instructions.)

OpenKIM IMs are uniquely identified by a KIM ID. The extended KIM ID consists of a human-readable prefix identifying the type of IM, authors, publication year, and supported species, separated by two underscores from the

KIM ID itself, which begins with an IM code (*MO* for a KIM Portable Model, and *SM* for a KIM Simulator Model) followed by a unique 12-digit code and a 3-digit version identifier. By convention SM prefixes begin with *Sim_* to readily identify them.

```
SW_StillingerWeber_1985_Si__MO_405512056662_005
Sim_LAMMPS_ReaxFF_StrachanVanDuinChakraborty_2003_CHNO__SM_107643900657_000
```

Each OpenKIM IM has a dedicated "Model Page" on OpenKIM providing all the information on the IM including a title, description, authorship and citation information, test and verification check results, visualizations of results, a wiki with documentation and user comments, and access to raw files, and other information. The URL for the Model Page is constructed from the extended KIM ID of the IM:

```
https://openkim.org/id/extended_KIM_ID
```

For example, for the Stillinger–Weber potential listed above the Model Page is located at:

https://openkim.org/id/SW_StillingerWeber_1985_Si__MO_405512056662_005

See the current list of KIM PMs and SMs archived in OpenKIM. This list is sorted by species and can be filtered to display only IMs for certain species combinations.

See Obtaining KIM Models to learn how to install a pre-build binary of the OpenKIM Repository of Models.

Note: It is also possible to locally install IMs not archived in OpenKIM, in which case their names do not have to conform to the KIM ID format.

Using OpenKIM IMs with LAMMPS

Two commands are employed when using OpenKIM IMs, one to select the IM and perform necessary initialization (*kim_init*), and the second to set up the IM for use by executing any necessary LAMMPS commands (*kim_interactions*). Both are required.

See the *examples/kim* directory for example input scripts that use KIM PMs and KIM SMs.

OpenKIM IM Initialization (*kim_init*)

The *kim_init* mode command must be issued **before** the simulation box is created (normally at the top of the file). This command sets the OpenKIM IM that will be used and may issue additional commands changing LAMMPS default settings that are required for using the selected IM (such as *units* or *atom_style*). If needed, those settings can be overridden, however, typically a script containing a *kim_init* command would not include *units* and *atom_style* commands.

The required arguments of *kim_init* are the *model* name of the IM to be used in the simulation (for an IM archived in OpenKIM this is its extended KIM ID, and the *user_units*, which are the LAMMPS *units style* used in the input script. (Any dimensioned numerical values in the input script and values read in from files are expected to be in the *user_units* system.)

The selected IM can be either a *KIM PM or a KIM SM*. For a KIM SM, the *kim_init* command verifies that the SM is designed to work with LAMMPS (and not another simulation code). In addition, the LAMMPS version used for defining the SM and the LAMMPS version being currently run are printed to help diagnose any incompatible changes to input script or command syntax between the two LAMMPS versions.

Based on the selected model *kim_init* may modify the *atom_style*. Some SMs have requirements for this setting. If this is the case, then *atom_style* will be set to the required style. Otherwise, the value is left unchanged (which in the absence of an *atom_style* command in the input script is the *default atom_style value*).

Regarding units, the *kim_init* command behaves in different ways depending on whether or not *unit conversion mode* is activated as indicated by the optional *unitarg* argument. If unit conversion mode is **not** active, then *user_units* must either match the required units of the IM or the IM must be able to adjust its units to match. (The latter is only possible with some KIM PMs; SMs can never adjust their units.) If a match is possible, the LAMMPS *units* command is called to set the units to *user_units*. If the match fails, the simulation is terminated with an error.

Here is an example of a LAMMPS script to compute the cohesive energy of a face-centered cubic (fcc) lattice for the Ercolessi and Adams (1994) potential for Al:

```
kim_init          EAM_Dynamo_ErcolessiAdams_1994_Al__MO_123629422045_005 metal
boundary          p p p
lattice           fcc 4.032
region            simbox block 0 1 0 1 0 1 units lattice
create_box        1 simbox
create_atoms      1 box
mass              1 26.981539
kim_interactions  Al
run               0
variable          Ec equal (pe/count(all))/${_u_energy}
print             "Cohesive Energy = ${EcJ} eV"
```

The above script will end with an error in the *kim_init* line if the IM is changed to another potential for Al that does not work with *metal* units. To address this *kim_init* offers the *unit_conversion_mode* as shown below. If unit conversion mode *is* active, then *kim_init* calls the LAMMPS *units* command to set the units to the IM's required or preferred units. Conversion factors between the IM's units and the *user_units* are defined for all *physical quantities* (mass, distance, etc.). (Note that converting to or from the "lj" unit style is not supported.) These factors are stored as *internal style variables* with the following standard names:

```
_u_mass
_u_distance
_u_time
_u_energy
_u_velocity
_u_force
_u_torque
_u_temperature
_u_pressure
_u_viscosity
_u_charge
_u_dipole
_u_efield
_u_density
```

If desired, the input script can be designed to work with these conversion factors so that the script will work without change with any OpenKIM IM. (This approach is used in the OpenKIM Testing Framework.) For example, the script given above for the cohesive energy of fcc Al can be rewritten to work with any IM regardless of units. The following script constructs an fcc lattice with a lattice parameter defined in meters, computes the total energy, and prints the cohesive energy in Joules regardless of the units of the IM.

```
kim_init          EAM_Dynamo_ErcolessiAdams_1994_Al__MO_123629422045_005 si unit_
↪conversion_mode
boundary          p p p
lattice           fcc 4.032e-10*${_u_distance}
region            simbox block 0 1 0 1 0 1 units lattice
create_box        1 simbox
create_atoms      1 box
mass              1 4.480134e-26*${_u_mass}
```

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```
kim_interactions Al
run              0
variable         Ec_in_J equal (pe/count(all))/${_u_energy}
print            "Cohesive Energy = ${Ec_in_J} J"
```

Note the multiplication by ${_u_distance} and ${_u_mass} to convert from SI units (specified in the *kim_init* command) to whatever units the IM uses (metal in this case), and the division by ${_u_energy} to convert from the IM's energy units to SI units (Joule). This script will work correctly for any IM for Al (KIM PM or SM) selected by the *kim_init* command.

Care must be taken to apply unit conversion to dimensional variables read in from a file. For example, if a configuration of atoms is read in from a dump file using the *read_dump* command, the following can be done to convert the box and all atomic positions to the correct units:

```
variable xyfinal equal xy*${_u_distance}
variable xzfinal equal xz*${_u_distance}
variable yzfinal equal yz*${_u_distance}
change_box all x scale ${_u_distance} &
                       y scale ${_u_distance} &
                       z scale ${_u_distance} &
                       xy final ${xyfinal} &
                       xz final ${xzfinal} &
                       yz final ${yzfinal} &
                       remap
```

Note: Unit conversion will only work if the conversion factors are placed in all appropriate places in the input script. It is up to the user to do this correctly.

OpenKIM IM Execution (*kim_interactions*)

The second and final step in using an OpenKIM IM is to execute the *kim_interactions* command. This command must be preceded by a *kim_init* command and a command that defines the number of atom types *N* (such as *create_box*). The *kim_interactions* command has one argument *typeargs*. This argument contains either a list of *N* chemical species, which defines a mapping between atom types in LAMMPS to the available species in the OpenKIM IM, or the keyword *fixed_types* for models that have a preset fixed mapping (i.e. the mapping between LAMMPS atom types and chemical species is defined by the model and cannot be changed). In the latter case, the user must consult the model documentation to see how many atom types there are and how they map to the chemical species.

For example, consider an OpenKIM IM that supports Si and C species. If the LAMMPS simulation has four atom types, where the first three are Si, and the fourth is C, the following *kim_interactions* command would be used:

```
kim_interactions Si Si Si C
```

Alternatively, for a model with a fixed mapping the command would be:

```
kim_interactions fixed_types
```

The *kim_interactions* command performs all the necessary steps to set up the OpenKIM IM selected in the *kim_init* command. The specific actions depend on whether the IM is a KIM PM or a KIM SM. For a KIM PM, a *pair_style kim* command is executed followed by the appropriate *pair_coeff* command. For example, for the Ercolessi and Adams (1994) KIM PM for Al set by the following commands:

```
kim_init EAM_Dynamo_ErcolessiAdams_1994_Al__MO_123629422045_005 metal
...
...  box specification lines skipped
...
kim_interactions Al
```

the *kim_interactions* command executes the following LAMMPS input commands:

```
pair_style kim EAM_Dynamo_ErcolessiAdams_1994_Al__MO_123629422045_005
pair_coeff * * Al
```

For a KIM SM, the generated input commands may be more complex and require that LAMMPS is built with the required packages included for the type of potential being used. The set of commands to be executed is defined in the SM specification file, which is part of the SM package. For example, for the Strachan et al. (2003) ReaxFF SM set by the following commands:

```
kim_init Sim_LAMMPS_ReaxFF_StrachanVanDuinChakraborty_2003_CHNO__SM_107643900657_000␣
↪real
...
...  box specification lines skipped
...
kim_interactions C H N O
```

the *kim_interactions* command executes the following LAMMPS input commands:

```
pair_style reax/c lmp_control safezone 2.0 mincap 100
pair_coeff * * ffield.reax.rdx C H N O
fix reaxqeq all qeq/reax 1 0.0 10.0 1.0e-6 param.qeq
```

Note that the files *lmp_control*, *ffield.reax.rdx* and *param.qeq* are specific to the Strachan et al. (2003) ReaxFF parameterization and are archived as part of the SM package in OpenKIM. Note also that parameters like cutoff radii and charge tolerances, which have an effect on IM predictions, are also included in the SM definition ensuring reproducibility.

Note: When using *kim_init* and *kim_interactions* to select and set up an OpenKIM IM, other LAMMPS commands for the same functions (such as pair_style, pair_coeff, bond_style, bond_coeff, fixes related to charge equilibration, etc.) should normally not appear in the input script.

Using OpenKIM Web Queries in LAMMPS (*kim_query*)

The *kim_query* command performs a web query to retrieve the predictions of an IM set by *kim_init* for material properties archived in OpenKIM.

Note: The *kim_query* command must be preceded by a *kim_init* command.

The syntax for the *kim_query* command is as follows:

```
kim_query variable formatarg query_function queryargs
```

The result of the query is stored in one or more *string style variables* as determined by the optional *formatarg* argument *documented above*. For the "list" setting of *formatarg* (or if *formatarg* is not specified), the result is returned as a space-separated list of values in *variable*. The *formatarg* keyword "split" separates the result values into individual variables

of the form *prefix_I*, where *prefix* is set to the *kim_query variable* argument and *I* ranges from 1 to the number of returned values. The number and order of the returned values is determined by the type of query performed. (Note that the "explicit" setting of *formatarg* is not supported by *kim_query*.)

Note: *kim_query* only supports queries that return a single result or an array of values. More complex queries that return a JSON structure are not currently supported. An attempt to use *kim_query* in such cases will generate an error.

The second required argument *query_function* is the name of the query function to be called (e.g. *get_lattice_constant_cubic*). All following *arguments* are parameters handed over to the web query in the format *keyword=value*, where *value* is always an array of one or more comma-separated items in brackets. The list of supported keywords and the type and format of their values depend on the query function used. The current list of query functions is available on the OpenKIM webpage at https://openkim.org/doc/usage/kim-query.

Note: All query functions require the *model* keyword, which identifies the IM whose predictions are being queried. This keyword is automatically generated by *kim_query* based on the IM set in *kim_init* and must not be specified as an argument to *kim_query*.

Note: Each *query_function* is associated with a default method (implemented as a KIM Test) used to compute this property. In cases where there are multiple methods in OpenKIM for computing a property, a *method* keyword can be provided to select the method of choice. See the query documentation to see which methods are available for a given *query function*.

kim_query Usage Examples and Further Clarifications

The data obtained by *kim_query* commands can be used as part of the setup or analysis phases of LAMMPS simulations. Some examples are given below.

Define an equilibrium fcc crystal

```
kim_init          EAM_Dynamo_ErcolessiAdams_1994_Al__MO_123629422045_005 metal
boundary          p p p
kim_query         a0 get_lattice_constant_cubic crystal=["fcc"] species=["Al"] units=[
↪"angstrom"]
lattice           fcc ${a0}
...
```

The *kim_query* command retrieves from OpenKIM the equilibrium lattice constant predicted by the Ercolessi and Adams (1994) potential for the fcc structure and places it in variable *a0*. This variable is then used on the next line to set up the crystal. By using *kim_query*, the user is saved the trouble and possible error of tracking this value down, or of having to perform an energy minimization to find the equilibrium lattice constant.

Note that in *unit_conversion_mode* the results obtained from a *kim_query* would need to be converted to the appropriate units system. For example, in the above script, the lattice command would need to be changed to: "lattice fcc ${a0}*${_u_distance}".

Define an equilibrium hcp crystal

```
kim_init          EAM_Dynamo_Mendelev_2007_Zr__MO_848899341753_000 metal
boundary          p p p
kim_query         latconst split get_lattice_constant_hexagonal crystal=["hcp"]␣
↪species=["Zr"] units=["angstrom"]
```

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```
variable          a0 equal latconst_1
variable          c0 equal latconst_2
variable          c_to_a equal ${c0}/${a0}
lattice           custom ${a0} a1 0.5 -0.866025 0 a2 0.5 0.866025 0 a3 0 0 ${c_to_a} &
                  basis 0.333333 0.666666 0.25 basis 0.666666 0.333333 0.75
...
```

In this case the *kim_query* returns two arguments (since the hexagonal close packed (hcp) structure has two independent lattice constants). The *formatarg* keyword "split" places the two values into the variables *latconst_1* and *latconst_2*. (These variables are created if they do not already exist.) For convenience the variables *a0* and *c0* are created in order to make the remainder of the input script more readable.

Define a crystal at finite temperature accounting for thermal expansion

```
kim_init          EAM_Dynamo_ErcolessiAdams_1994_Al__MO_123629422045_005 metal
boundary          p p p
kim_query         a0 get_lattice_constant_cubic crystal=["fcc"] species=["Al"] units=[
↪"angstrom"]
kim_query         alpha get_linear_thermal_expansion_coefficient_cubic  crystal=["fcc
↪"] species=["Al"] units=["1/K"] temperature=[293.15] temperature_units=["K"]
variable          DeltaT equal 300
lattice           fcc ${a0}*${alpha}*${DeltaT}
...
```

As in the previous example, the equilibrium lattice constant is obtained for the Ercolessi and Adams (1994) potential. However, in this case the crystal is scaled to the appropriate lattice constant at room temperature (293.15 K) by using the linear thermal expansion constant predicted by the potential.

Note: When passing numerical values as arguments (as in the case of the temperature in the above example) it is also possible to pass a tolerance indicating how close to the value is considered a match. If no tolerance is passed a default value is used. If multiple results are returned (indicating that the tolerance is too large), *kim_query* will return an error. See the query documentation to see which numerical arguments and tolerances are available for a given *query function*.

Compute defect formation energy

```
kim_init          EAM_Dynamo_ErcolessiAdams_1994_Al__MO_123629422045_005 metal
...
... Build fcc crystal containing some defect and compute the total energy
... which is stored in the variable *Etot*
...
kim_query         Ec get_cohesive_energy_cubic crystal=["fcc"] species=["Al"] units=[
↪"eV"]
variable          Eform equal ${Etot} - count(all)*${Ec}
...
```

The defect formation energy *Eform* is computed by subtracting from *Etot* the ideal fcc cohesive energy of the atoms in the system obtained from OpenKIM for the Ercolessi and Adams (1994) potential.

Note: *kim_query* commands return results archived in OpenKIM. These results are obtained using programs for computing material properties (KIM Tests and KIM Test Drivers) that were contributed to OpenKIM. In order to give credit to Test developers, the number of times results from these programs are queried is tracked. No other information about the nature of the query or its source is recorded.

Accessing KIM Model Parameters from LAMMPS (*kim_param*)

All IMs are functional forms containing a set of parameters. The values of these parameters are typically selected to best reproduce a training set of quantum mechanical calculations or available experimental data. For example, a Lennard-Jones potential intended to model argon might have the values of its two parameters, epsilon and sigma, fit to the dimer dissociation energy or thermodynamic properties at a critical point of the phase diagram.

Normally a user employing an IM should not modify its parameters since, as noted above, these are selected to reproduce material properties. However, there are cases where accessing and modifying IM parameters is desired, such as for assessing uncertainty, fitting an IM, or working with an ensemble of IMs. As explained *above*, IMs archived in OpenKIM are either Portable Models (PMs) or Simulator Models (SMs). KIM PMs are complete independent implementations of an IM, whereas KIM SMs are wrappers to an IM implemented within LAMMPS. Two different mechanisms are provided for accessing IM parameters in these two cases:

- For a KIM PM, the *kim_param* command can be used to *get* and *set* the values of the PM's parameters as explained below.
- For a KIM SM, the user should consult the documentation page for the specific IM and follow instructions there for how to modify its parameters (if possible).

The *kim_param get* and *kim_param set* commands provide an interface to access and change the parameters of a KIM PM that "publishes" its parameters and makes them publicly available (see the KIM API documentation for details).

Note: The *kim_param get/set* commands must be preceded by *kim_init*. The *kim_param set* command must additionally be preceded by a *kim_interactions* command (or alternatively by a *pair_style kim* and *pair_coeff* commands). The *kim_param set* command may be used wherever a *pair_coeff* command may occur.

The syntax for the *kim_param* command is as follows:

```
kim_param get param_name index_range variable formatarg
kim_param set param_name index_range values
```

Here, *param_name* is the name of a KIM PM parameter (which is published by the PM and available for access). The specific string used to identify a parameter is defined by the PM. For example, for the Stillinger–Weber (SW) potential in OpenKIM, the parameter names are *A, B, p, q, sigma, gamma, cutoff, lambda, costheta0*.

Note: The list of all the parameters that a PM exposes for access/mutation are automatically written to the lammps log file when *kim_init* is called.

Each published parameter of a KIM PM takes the form of an array of numerical values. The array can contain one element for a single-valued parameter, or a set of values. For example, the multispecies SW potential for the Zn-Cd-Hg-S-Se-Te system has the same parameter names as the single-species SW potential, but each parameter array contains 21 entries that correspond to the parameter values used for each pairwise combination of the model's six supported species (this model does not have parameters specific to individual ternary combinations of its supported species).

The *index_range* argument may either be an integer referring to a specific element within the array associated with the parameter specified by *param_name*, or a pair of integers separated by a colon that refer to a slice of this array. In both cases, one-based indexing is used to refer to the entries of the array.

The result of a *get* operation for a specific *index_range* is stored in one or more *LAMMPS string style variables* as determined by the optional *formatarg* argument *documented above.* If not specified, the default for *formatarg* is "explicit" for the *kim_param* command.

For the case where the result is an array with multiple values (i.e. *index_range* contains a range), the optional "split" or "explicit" *formatarg* keywords can be used to separate the results into multiple variables; see the examples below. Multiple parameters can be retrieved with a single call to *kim_param get* by repeating the argument list following *get*.

For a *set* operation, the *values* argument contains the new value(s) for the element(s) of the parameter specified by *index_range*. For the case where multiple values are being set, *values* contains a set of values separated by spaces. Multiple parameters can be set with a single call to *kim_param set* by repeating the argument list following *set*.

kim_param Usage Examples and Further Clarifications

Examples of getting and setting KIM PM parameters with further clarifications are provided below.

Getting a scalar parameter

```
kim_init          SW_StillingerWeber_1985_Si__MO_405512056662_005 metal
...
kim_param         get A 1 VARA
```

In this case, the value of the SW *A* parameter is retrieved and placed in the LAMMPS variable *VARA*. The variable *VARA* can be used in the remainder of the input script in the same manner as any other LAMMPS variable.

Getting multiple scalar parameters with a single call

```
kim_init          SW_StillingerWeber_1985_Si__MO_405512056662_005 metal
...
kim_param         get A 1 VARA B 1 VARB
```

This retrieves the *A* and *B* parameters of the SW potential and stores them in the LAMMPS variables *VARA* and *VARB*.

Getting a range of values from a parameter

There are several options when getting a range of values from a parameter determined by the *formatarg* argument.

```
kim_init          SW_ZhouWardMartin_2013_CdTeZnSeHgS__MO_503261197030_002 metal
...
kim_param         get lambda 7:9 LAM_TeTe LAM_TeZn LAM_TeSe
```

In this case, *formatarg* is not specified and therefore the default "explicit" mode is used. (The behavior would be the same if the word *explicit* were added after *LAM_TeSe*.) Elements 7, 8 and 9 of parameter lambda retrieved by the *get* operation are placed in the LAMMPS variables *LAM_TeTe*, *LAM_TeZn* and *LAM_TeSe*, respectively.

Note: In the above example, elements 7–9 of the lambda parameter correspond to Te-Te, Te-Zm and Te-Se interactions. This can be determined by visiting the model page for the specified potential and looking at its parameter file linked to at the bottom of the page (file with .param ending) and consulting the README documentation provided with the driver for the PM being used. A link to the driver is provided at the top of the model page.

```
kim_init          SW_ZhouWardMartin_2013_CdTeZnSeHgS__MO_503261197030_002 metal
...
kim_param         get lambda 15:17 LAMS list
variable          LAM_VALUE index ${LAMS}
label             loop_on_lambda
...
... do something with current value of lambda
...
next              LAM_VALUE
jump              SELF loop_on_lambda
```

In this case, the "list" mode of *formatarg* is used. The result of the *get* operation is stored in the LAMMPS variable *LAMS* as a string containing the three retrieved values separated by spaces, e.g "1.0 2.0 3.0". This can be used in LAMMPS with an *index* variable to access the values one at a time within a loop as shown in the example. At each iteration of the loop *LAM_VALUE* contains the current value of lambda.

```
kim_init          SW_ZhouWardMartin_2013_CdTeZnSeHgS__MO_503261197030_002 metal
...
kim_param         get lambda 15:17 LAM split
```

In this case, the "split" mode of *formatarg* is used. The three values retrieved by the *get* operation are stored in the three LAMMPS variables *LAM_15*, *LAM_16* and *LAM_17*. The provided name "LAM" is used as prefix and the location in the lambda array is appended to create the variable names.

Setting a scalar parameter

```
kim_init          SW_StillingerWeber_1985_Si__MO_405512056662_005 metal
...
kim_interactions Si
kim_param         set gamma 1 2.6
```

Here, the SW potential's gamma parameter is set to 2.6. Note that the *get* and *set* commands work together, so that a *get* following a *set* operation will return the new value that was set. For example:

```
...
kim_interactions Si
kim_param         get gamma 1 ORIG_GAMMA
kim_param         set gamma 1 2.6
kim_param         get gamma 1 NEW_GAMMA
...
print             "original gamma = ${ORIG_GAMMA}, new gamma = ${NEW_GAMMA}"
```

Here, *ORIG_GAMMA* will contain the original gamma value for the SW potential, while *NEW_GAMMA* will contain the value 2.6.

Setting multiple scalar parameters with a single call

```
kim_init          SW_ZhouWardMartin_2013_CdTeZnSeHgS__MO_503261197030_002 metal
...
kim_interactions Cd Te
variable         VARG equal 2.6
variable         VARS equal 2.0951
kim_param        set gamma 1 ${VARG} sigma 3 ${VARS}
```

In this case, the first element of the *gamma* parameter and third element of the *sigma* parameter are set to 2.6 and 2.0951, respectively. This example also shows how LAMMPS variables can be used when setting parameters.

Setting a range of values of a parameter

```
kim_init          SW_ZhouWardMartin_2013_CdTeZnSeHgS__MO_503261197030_002 metal
...
kim_interactions Cd Te Zn Se Hg S
kim_param         set sigma 2:6 2.35214 2.23869 2.04516 2.43269 1.80415
```

In this case, elements 2 through 6 of the parameter *sigma* are set to the values 2.35214, 2.23869, 2.04516, 2.43269 and 1.80415 in order.

Citation of OpenKIM IMs

When publishing results obtained using OpenKIM IMs researchers are requested to cite the OpenKIM project *(Tadmor)*, KIM API *(Elliott)*, and the specific IM codes used in the simulations, in addition to the relevant scientific references for the IM. The citation format for an IM is displayed on its page on OpenKIM along with the corresponding BibTex file, and is automatically added to the LAMMPS *log.cite* file.

Citing the IM software (KIM infrastructure and specific PM or SM codes) used in the simulation gives credit to the researchers who developed them and enables open source efforts like OpenKIM to function.

15.64.4 Restrictions

The set of *kim_commands* is part of the KIM package. It is only enabled if LAMMPS is built with that package. A requirement for the KIM package, is the KIM API library that must be downloaded from the OpenKIM website and installed before LAMMPS is compiled. When installing LAMMPS from binary, the kim-api package is a dependency that is automatically downloaded and installed. See the KIM section of the *Packages details* for details.

Furthermore, when using *kim_commands* to run KIM SMs, any packages required by the native potential being used or other commands or fixes that it invokes must be installed.

15.64.5 Related commands

pair_style kim

(Tadmor) Tadmor, Elliott, Sethna, Miller and Becker, JOM, 63, 17 (2011). doi: https://doi.org/10.1007/s11837-011-0102-6

(Elliott) Elliott, Tadmor and Bernstein, https://openkim.org/kim-api (2011) doi: https://doi.org/10.25950/FF8F563A

15.65 kspace_modify command

15.65.1 Syntax

```
kspace_modify keyword value ...
```

- one or more keyword/value pairs may be listed
- keyword = *collective* or *compute* or *cutoff/adjust* or *diff* or *disp/auto* or *fftbench* or *force/disp/kspace* or *force/disp/real* or *force* or *gewald/disp* or *gewald* or *kmax/ewald* or *mesh* or *minorder* or *mix/disp* or *order/disp* or *order* or *overlap* or *scafacos* or *slab* or *splittol*

```
collective value = yes or no
compute value = yes or no
cutoff/adjust value = yes or no
diff value = ad or ik = 2 or 4 FFTs for PPPM in smoothed or non-smoothed␣
↪mode
disp/auto value = yes or no
fftbench value = yes or no
force/disp/real value = accuracy (force units)
force/disp/kspace value = accuracy (force units)
force value = accuracy (force units)
```

```
gewald value = rinv (1/distance units)
  rinv = G-ewald parameter for Coulombics
gewald/disp value = rinv (1/distance units)
  rinv = G-ewald parameter for dispersion
kmax/ewald value = kx ky kz
  kx,ky,kz = number of Ewald sum kspace vectors in each dimension
mesh value = x y z
  x,y,z = grid size in each dimension for long-range Coulombics
mesh/disp value = x y z
  x,y,z = grid size in each dimension for 1/r^6 dispersion
minorder value = M
  M = min allowed extent of Gaussian when auto-adjusting to minimize grid␣
↪communication
mix/disp value = pair or geom or none
order value = N
  N = extent of Gaussian for PPPM or MSM mapping of charge to grid
order/disp value = N
  N = extent of Gaussian for PPPM mapping of dispersion term to grid
overlap = yes or no = whether the grid stencil for PPPM is allowed to␣
↪overlap into more than the nearest-neighbor processor
pressure/scalar value = yes or no
scafacos values = option value1 value2 ...
  option = tolerance
    value = energy or energy_rel or field or field_rel or potential or␣
↪potential_rel
  option = fmm_tuning
    value = 0 or 1
slab value = volfactor or nozforce
  volfactor = ratio of the total extended volume used in the
    2d approximation compared with the volume of the simulation domain
  nozforce turns off kspace forces in the z direction
splittol value = tol
  tol = relative size of two eigenvalues (see discussion below)
```

15.65.2 Examples

```
kspace_modify mesh 24 24 30 order 6
kspace_modify slab 3.0
kspace_modify scafacos tolerance energy
```

15.65.3 Description

Set parameters used by the kspace solvers defined by the *kspace_style* command. Not all parameters are relevant to all kspace styles.

The *collective* keyword applies only to PPPM. It is set to *no* by default, except on IBM BlueGene machines. If this option is set to *yes*, LAMMPS will use MPI collective operations to remap data for 3d-FFT operations instead of the default point-to-point communication. This is faster on IBM BlueGene machines, and may also be faster on other machines if they have an efficient implementation of MPI collective operations and adequate hardware.

The *compute* keyword allows Kspace computations to be turned off, even though a *kspace_style* is defined. This is not useful for running a real simulation, but can be useful for debugging purposes or for computing only partial forces that do not include the Kspace contribution. You can also do this by simply not defining a *kspace_style*, but a Kspace-compatible *pair_style* requires a kspace style to be defined. This keyword gives you that option.

The *cutoff/adjust* keyword applies only to MSM. If this option is turned on, the Coulombic cutoff will be automatically adjusted at the beginning of the run to give the desired estimated error. Other cutoffs such as LJ will not be affected. If the grid is not set using the *mesh* command, this command will also attempt to use the optimal grid that minimizes cost using an estimate given by *(Hardy)*. Note that this cost estimate is not exact, somewhat experimental, and still may not yield the optimal parameters.

The *diff* keyword specifies the differentiation scheme used by the PPPM method to compute forces on particles given electrostatic potentials on the PPPM mesh. The *ik* approach is the default for PPPM and is the original formulation used in *(Hockney)*. It performs differentiation in Kspace, and uses 3 FFTs to transfer each component of the computed fields back to real space for total of 4 FFTs per timestep.

The analytic differentiation *ad* approach uses only 1 FFT to transfer information back to real space for a total of 2 FFTs per timestep. It then performs analytic differentiation on the single quantity to generate the 3 components of the electric field at each grid point. This is sometimes referred to as "smoothed" PPPM. This approach requires a somewhat larger PPPM mesh to achieve the same accuracy as the *ik* method. Currently, only the *ik* method (default) can be used for a triclinic simulation cell with PPPM. The *ad* method is always used for MSM.

Note: Currently, not all PPPM styles support the *ad* option. Support for those PPPM variants will be added later.

The *disp/auto* option controls whether the pppm/disp is allowed to generate PPPM parameters automatically. If set to *no*, parameters have to be specified using the *gewald/disp*, *mesh/disp*, *force/disp/real* or *force/disp/kspace* keywords, or the code will stop with an error message. When this option is set to *yes*, the error message will not appear and the simulation will start. For a typical application, using the automatic parameter generation will provide simulations that are either inaccurate or slow. Using this option is thus not recommended. For guidelines on how to obtain good parameters, see the *How-To* discussion.

The *fftbench* keyword applies only to PPPM. It is off by default. If this option is turned on, LAMMPS will perform a short FFT benchmark computation and report its timings, and will thus finish a some seconds later than it would if this option were off.

The *force/disp/real* and *force/disp/kspace* keywords set the force accuracy for the real and space computations for the dispersion part of pppm/disp. As shown in *(Isele-Holder)*, optimal performance and accuracy in the results is obtained when these values are different.

The *force* keyword overrides the relative accuracy parameter set by the *kspace_style* command with an absolute accuracy. The accuracy determines the RMS error in per-atom forces calculated by the long-range solver and is thus specified in force units. A negative value for the accuracy setting means to use the relative accuracy parameter. The accuracy setting is used in conjunction with the pairwise cutoff to determine the number of K-space vectors for style *ewald*, the FFT grid size for style *pppm*, or the real space grid size for style *msm*.

The *gewald* keyword sets the value of the Ewald or PPPM G-ewald parameter for charge as *rinv* in reciprocal distance units. Without this setting, LAMMPS chooses the parameter automatically as a function of cutoff, precision, grid spacing, etc. This means it can vary from one simulation to the next which may not be desirable for matching a KSpace solver to a pre-tabulated pairwise potential. This setting can also be useful if Ewald or PPPM fails to choose a good grid spacing and G-ewald parameter automatically. If the value is set to 0.0, LAMMPS will choose the G-ewald parameter automatically. MSM does not use the *gewald* parameter.

The *gewald/disp* keyword sets the value of the Ewald or PPPM G-ewald parameter for dispersion as *rinv* in reciprocal distance units. It has the same meaning as the *gewald* setting for Coulombics.

The *kmax/ewald* keyword sets the number of kspace vectors in each dimension for kspace style *ewald*. The three values must be positive integers, or else (0,0,0), which unsets the option. When this option is not set, the Ewald sum scheme chooses its own kspace vectors, consistent with the user-specified accuracy and pairwise cutoff. In any case, if kspace style *ewald* is invoked, the values used are printed to the screen and the log file at the start of the run.

The *mesh* keyword sets the grid size for kspace style *pppm* or *msm*. In the case of PPPM, this is the FFT mesh, and each dimension must be factorizable into powers of 2, 3, and 5. In the case of MSM, this is the finest scale real-space mesh, and each dimension must be factorizable into powers of 2. When this option is not set, the PPPM or MSM solver chooses its own grid size, consistent with the user-specified accuracy and pairwise cutoff. Values for x,y,z of 0,0,0 unset the option.

The *mesh/disp* keyword sets the grid size for kspace style *pppm/disp*. This is the FFT mesh for long-range dispersion and ach dimension must be factorizable into powers of 2, 3, and 5. When this option is not set, the PPPM solver chooses its own grid size, consistent with the user-specified accuracy and pairwise cutoff. Values for x,y,z of 0,0,0 unset the option.

The *minorder* keyword allows LAMMPS to reduce the *order* setting if necessary to keep the communication of ghost grid point limited to exchanges between nearest-neighbor processors. See the discussion of the *overlap* keyword for details. If the *overlap* keyword is set to *yes*, which is the default, this is never needed. If it set to *no* and overlap occurs, then LAMMPS will reduce the order setting, one step at a time, until the ghost grid overlap only extends to nearest neighbor processors. The *minorder* keyword limits how small the *order* setting can become. The minimum allowed value for PPPM is 2, which is the default. If *minorder* is set to the same value as *order* then no reduction is allowed, and LAMMPS will generate an error if the grid communication is non-nearest-neighbor and *overlap* is set to *no*. The *minorder* keyword is not currently supported in MSM.

The *mix/disp* keyword selects the mixing rule for the dispersion coefficients. With *pair*, the dispersion coefficients of unlike types are computed as indicated with *pair_modify*. With *geom*, geometric mixing is enforced on the dispersion coefficients in the kspace coefficients. When using the arithmetic mixing rule, this will speed-up the simulations but introduces some error in the force computations, as shown in *(Wennberg)*. With *none*, it is assumed that no mixing rule is applicable. Splitting of the dispersion coefficients will be performed as described in *(Isele-Holder)*.

This splitting can be influenced with the *splittol* keywords. Only the eigenvalues that are larger than tol compared to the largest eigenvalues are included. Using this keywords the original matrix of dispersion coefficients is approximated. This leads to faster computations, but the accuracy in the reciprocal space computations of the dispersion part is decreased.

The *order* keyword determines how many grid spacings an atom's charge extends when it is mapped to the grid in kspace style *pppm* or *msm*. The default for this parameter is 5 for PPPM and 8 for MSM, which means each charge spans 5 or 8 grid cells in each dimension, respectively. For the LAMMPS implementation of MSM, the order can range from 4 to 10 and must be even. For PPPM, the minimum allowed setting is 2 and the maximum allowed setting is 7. The larger the value of this parameter, the smaller that LAMMPS will set the grid size, to achieve the requested accuracy. Conversely, the smaller the order value, the larger the grid size will be. Note that there is an inherent trade-off involved: a small grid will lower the cost of FFTs or MSM direct sum, but a larger order parameter will increase the cost of interpolating charge/fields to/from the grid.

The PPPM order parameter may be reset by LAMMPS when it sets up the FFT grid if the implied grid stencil extends beyond the grid cells owned by neighboring processors. Typically this will only occur when small problems are run on large numbers of processors. A warning will be generated indicating the order parameter is being reduced to allow LAMMPS to run the problem. Automatic adjustment of the order parameter is not supported in MSM.

The *order/disp* keyword determines how many grid spacings an atom's dispersion term extends when it is mapped to the grid in kspace style *pppm/disp*. It has the same meaning as the *order* setting for Coulombics.

The *overlap* keyword can be used in conjunction with the *minorder* keyword with the PPPM styles to adjust the amount of communication that occurs when values on the FFT grid are exchanged between processors. This communication is distinct from the communication inherent in the parallel FFTs themselves, and is required because processors interpolate charge and field values using grid point values owned by neighboring processors (i.e. ghost point communication). If the *overlap* keyword is set to *yes* then this communication is allowed to extend beyond nearest-neighbor processors, e.g. when using lots of processors on a small problem. If it is set to *no* then the communication will be limited to nearest-neighbor processors and the *order* setting will be reduced if necessary, as explained by the *minorder* keyword discussion. The *overlap* keyword is always set to *yes* in MSM.

The *pressure/scalar* keyword applies only to MSM. If this option is turned on, only the scalar pressure (i.e. (Pxx + Pyy + Pzz)/3.0) will be computed, which can be used, for example, to run an isotropic barostat. Computing the full pressure tensor with MSM is expensive, and this option provides a faster alternative. The scalar pressure is computed using a relationship between the Coulombic energy and pressure *(Hummer)* instead of using the virial equation. This option cannot be used to access individual components of the pressure tensor, to compute per-atom virial, or with suffix kspace/pair styles of MSM, like OMP or GPU.

The *scafacos* keyword is used for settings that are passed to the ScaFaCoS library when using *kspace_style scafacos*.

The *tolerance* option affects how the *accuracy* specified with the *kspace_style* command is interpreted by ScaFaCoS. The following values may be used:

- energy = absolute accuracy in total Coulombic energy
- energy_rel = relative accuracy in total Coulombic energy
- potential = absolute accuracy in total Coulombic potential
- potential_rel = relative accuracy in total Coulombic potential
- field = absolute accuracy in electric field
- field_rel = relative accuracy in electric field

The values with suffix _rel indicate the tolerance is a relative tolerance; the other values impose an absolute tolerance on the given quantity. Absolute tolerance in this case means, that for a given quantity q and a given absolute tolerance of t_a the result should be between q-t_a and q+t_a. For a relative tolerance t_r the relative error should not be greater than t_r, i.e. abs(1 - (result/q)) < t_r. As a consequence of this, the tolerance type should be checked, when

performing computations with a high absolute field / energy. E.g. if the total energy in the system is 1000000.0 an absolute tolerance of 1e-3 would mean that the result has to be between 999999.999 and 1000000.001, which would be equivalent to a relative tolerance of 1e-9.

The energy and energy_rel values, set a tolerance based on the total Coulombic energy of the system. The potential and potential_rel set a tolerance based on the per-atom Coulombic energy. The field and field_rel tolerance types set a tolerance based on the electric field values computed by ScaFaCoS. Since per-atom forces are derived from the per-atom electric field, this effectively sets a tolerance on the forces, similar to other LAMMPS KSpace styles, as explained on the *kspace_style* doc page.

Note that not all ScaFaCoS solvers support all tolerance types. These are the allowed values for each method:

- fmm = energy and energy_rel
- p2nfft = field (1d-,2d-,3d-periodic systems) or potential (0d-periodic)
- p3m = field
- ewald = field
- direct = has no tolerance tuning

If the tolerance type is not changed, the default values for the tolerance type are the first values in the above list, e.g. energy is the default tolerance type for the fmm solver.

The *fmm_tuning* option is only relevant when using the FMM method. It activates (value=1) or deactivates (value=0) an internal tuning mechanism for the FMM solver. The tuning operation runs sequentially and can be very time-consuming. Usually it is not needed for systems with a homogeneous charge distribution. The default for this option is therefore *0*. The FMM internal tuning is performed once, when the solver is set up.

The *slab* keyword allows an Ewald or PPPM solver to be used for a systems that are periodic in x,y but non-periodic in z - a *boundary* setting of "boundary p p f". This is done by treating the system as if it were periodic in z, but inserting empty volume between atom slabs and removing dipole inter-slab interactions so that slab-slab interactions are effectively turned off. The volfactor value sets the ratio of the extended dimension in z divided by the actual dimension in z. The recommended value is 3.0. A larger value is inefficient; a smaller value introduces unwanted slab-slab interactions. The use of fixed boundaries in z means that the user must prevent particle migration beyond the initial z-bounds, typically by providing a wall-style fix. The methodology behind the *slab* option is explained in the paper by *(Yeh)*. The *slab* option is also extended to non-neutral systems *(Ballenegger)*.

An alternative slab option can be invoked with the *nozforce* keyword in lieu of the volfactor. This turns off all kspace forces in the z direction. The *nozforce* option is not supported by MSM. For MSM, any combination of periodic, non-periodic, or shrink-wrapped boundaries can be set using *boundary* (the slab approximation in not needed). The *slab* keyword is not currently supported by Ewald or PPPM when using a triclinic simulation cell. The slab correction has also been extended to point dipole interactions *(Klapp)* in *kspace_style* *ewald/disp*, *ewald/dipole*, and *pppm/dipole*.

Note: If you wish to apply an electric field in the Z-direction, in conjunction with the *slab* keyword, you should do it by adding explicit charged particles to the +/- Z surfaces. If you do it via the *fix efield* command, it will not give the correct dielectric constant due to the Yeh/Berkowitz *(Yeh)* correction not being compatible with how *fix efield* works.

The *force/disp/real* and *force/disp/kspace* keywords set the force accuracy for the real and space computations for the dispersion part of pppm/disp. As shown in *(Isele-Holder)*, optimal performance and accuracy in the results is obtained when these values are different.

The *disp/auto* option controls whether the pppm/disp is allowed to generate PPPM parameters automatically. If set to *no*, parameters have to be specified using the *gewald/disp*, *mesh/disp*, *force/disp/real* or *force/disp/kspace* keywords, or the code will stop with an error message. When this option is set to *yes*, the error message will not appear and

the simulation will start. For a typical application, using the automatic parameter generation will provide simulations that are either inaccurate or slow. Using this option is thus not recommended. For guidelines on how to obtain good parameters, see the *Howto dispersion* doc page.

15.65.4 Restrictions

none

15.65.5 Related commands

kspace_style, *boundary*

15.65.6 Default

The option defaults are mesh = mesh/disp = 0 0 0, order = order/disp = 5 (PPPM), order = 10 (MSM), minorder = 2, overlap = yes, force = -1.0, gewald = gewald/disp = 0.0, slab = 1.0, compute = yes, cutoff/adjust = yes (MSM), pressure/scalar = yes (MSM), fftbench = no (PPPM), diff = ik (PPPM), mix/disp = pair, force/disp/real = -1.0, force/disp/kspace = -1.0, split = 0, tol = 1.0e-6, and disp/auto = no. For pppm/intel, order = order/disp = 7. For scafacos settings, the scafacos tolerance option depends on the method chosen, as documented above. The scafacos fmm_tuning default = 0.

(Hockney) Hockney and Eastwood, Computer Simulation Using Particles, Adam Hilger, NY (1989).

(Yeh) Yeh and Berkowitz, J Chem Phys, 111, 3155 (1999).

(Ballenegger) Ballenegger, Arnold, Cerda, J Chem Phys, 131, 094107 (2009).

(Klapp) Klapp, Schoen, J Chem Phys, 117, 8050 (2002).

(Hardy) David Hardy thesis: Multilevel Summation for the Fast Evaluation of Forces for the Simulation of Biomolecules, University of Illinois at Urbana-Champaign, (2006).

(Hummer) Hummer, Gronbech-Jensen, Neumann, J Chem Phys, 109, 2791 (1998)

(Isele-Holder) Isele-Holder, Mitchell, Hammond, Kohlmeyer, Ismail, J Chem Theory Comput, 9, 5412 (2013).

(Wennberg) Wennberg, Murtola, Hess, Lindahl, J Chem Theory Comput, 9, 3527 (2013).

15.66 kspace_style command

15.66.1 Syntax

```
kspace_style style value
```

- style = *none* or *ewald* or *ewald/dipole* or *ewald/dipole/spin* or *ewald/disp* or *ewald/omp* or *pppm* or *pppm/cg* or *pppm/disp* or *pppm/tip4p* or *pppm/stagger* or *pppm/disp/tip4p* or *pppm/gpu* or *pppm/intel* or *pppm/disp/intel* or *pppm/kk* or *pppm/omp* or *pppm/cg/omp* or *pppm/disp/tip4p/omp* or *pppm/tip4p/omp* or *msm* or *msm/cg* or *msm/omp* or *msm/cg/omp* or *scafacos*

```
none value = none
ewald value = accuracy
  accuracy = desired relative error in forces
ewald/dipole value = accuracy
  accuracy = desired relative error in forces
ewald/dipole/spin value = accuracy
  accuracy = desired relative error in forces
ewald/disp value = accuracy
  accuracy = desired relative error in forces
ewald/omp value = accuracy
  accuracy = desired relative error in forces
pppm value = accuracy
  accuracy = desired relative error in forces
pppm/cg values = accuracy (smallq)
  accuracy = desired relative error in forces
  smallq = cutoff for charges to be considered (optional) (charge units)
pppm/dipole value = accuracy
  accuracy = desired relative error in forces
pppm/dipole/spin value = accuracy
  accuracy = desired relative error in forces
pppm/disp value = accuracy
  accuracy = desired relative error in forces
pppm/tip4p value = accuracy
  accuracy = desired relative error in forces
pppm/disp/tip4p value = accuracy
  accuracy = desired relative error in forces
pppm/gpu value = accuracy
  accuracy = desired relative error in forces
pppm/intel value = accuracy
  accuracy = desired relative error in forces
pppm/disp/intel value = accuracy
  accuracy = desired relative error in forces
pppm/kk value = accuracy
  accuracy = desired relative error in forces
pppm/omp value = accuracy
  accuracy = desired relative error in forces
pppm/cg/omp values = accuracy (smallq)
  accuracy = desired relative error in forces
  smallq = cutoff for charges to be considered (optional) (charge units)
pppm/disp/omp value = accuracy
  accuracy = desired relative error in forces
pppm/tip4p/omp value = accuracy
  accuracy = desired relative error in forces
pppm/disp/tip4p/omp value = accuracy
  accuracy = desired relative error in forces
pppm/stagger value = accuracy
  accuracy = desired relative error in forces
msm value = accuracy
  accuracy = desired relative error in forces
msm/cg value = accuracy (smallq)
  accuracy = desired relative error in forces
  smallq = cutoff for charges to be considered (optional) (charge units)
msm/omp value = accuracy
  accuracy = desired relative error in forces
```

```
msm/cg/omp value = accuracy (smallq)
  accuracy = desired relative error in forces
  smallq = cutoff for charges to be considered (optional) (charge units)
scafacos values = method accuracy
  method = fmm or p2nfft or p3m or ewald or direct
  accuracy = desired relative error in forces
```

15.66.2 Examples

```
kspace_style pppm 1.0e-4
kspace_style pppm/cg 1.0e-5 1.0e-6
kspace style msm 1.0e-4
kspace style scafacos fmm 1.0e-4
kspace_style none
```

15.66.3 Description

Define a long-range solver for LAMMPS to use each timestep to compute long-range Coulombic interactions or long-range $1/r^6$ interactions. Most of the long-range solvers perform their computation in K-space, hence the name of this command.

When such a solver is used in conjunction with an appropriate pair style, the cutoff for Coulombic or $1/r^N$ interactions is effectively infinite. If the Coulombic case, this means each charge in the system interacts with charges in an infinite array of periodic images of the simulation domain.

Note that using a long-range solver requires use of a matching *pair style* to perform consistent short-range pairwise calculations. This means that the name of the pair style contains a matching keyword to the name of the KSpace style, as in this table:

Pair style	KSpace style
coul/long	ewald or pppm
coul/msm	msm
lj/long or buck/long	disp (for dispersion)
tip4p/long	tip4p

The *ewald* style performs a standard Ewald summation as described in any solid-state physics text.

The *ewald/disp* style adds a long-range dispersion sum option for $1/r^6$ potentials and is useful for simulation of interfaces *(Veld)*. It also performs standard Coulombic Ewald summations, but in a more efficient manner than the *ewald* style. The $1/r^6$ capability means that Lennard-Jones or Buckingham potentials can be used without a cutoff, i.e. they become full long-range potentials. The *ewald/disp* style can also be used with point-dipoles, see *(Toukmaji)*.

The *ewald/dipole* style adds long-range standard Ewald summations for dipole-dipole interactions, see *(Toukmaji)*.

The *ewald/dipole/spin* style adds long-range standard Ewald summations for magnetic dipole-dipole interactions between magnetic spins.

The *pppm* style invokes a particle-particle particle-mesh solver *(Hockney)* which maps atom charge to a 3d mesh, uses 3d FFTs to solve Poisson's equation on the mesh, then interpolates electric fields on the mesh points back to the atoms. It is closely related to the particle-mesh Ewald technique (PME) *(Darden)* used in AMBER and CHARMM. The cost

of traditional Ewald summation scales as $N^{\frac{3}{2}}$ where N is the number of atoms in the system. The PPPM solver scales as $N \log N$ due to the FFTs, so it is almost always a faster choice *(Pollock)*.

The *pppm/cg* style is identical to the *pppm* style except that it has an optimization for systems where most particles are uncharged. Similarly the *msm/cg* style implements the same optimization for *msm*. The optional *smallq* argument defines the cutoff for the absolute charge value which determines whether a particle is considered charged or not. Its default value is 1.0e-5.

The *pppm/dipole* style invokes a particle-particle particle-mesh solver for dipole-dipole interactions, following the method of *(Cerda)*.

The *pppm/dipole/spin* style invokes a particle-particle particle-mesh solver for magnetic dipole-dipole interactions between magnetic spins.

The *pppm/tip4p* style is identical to the *pppm* style except that it adds a charge at the massless 4th site in each TIP4P water molecule. It should be used with *pair styles* with a *tip4p/long* in their style name.

The *pppm/stagger* style performs calculations using two different meshes, one shifted slightly with respect to the other. This can reduce force aliasing errors and increase the accuracy of the method for a given mesh size. Or a coarser mesh can be used for the same target accuracy, which saves CPU time. However, there is a trade-off since FFTs on two meshes are now performed which increases the computation required. See *(Cerutti)*, *(Neelov)*, and *(Hockney)* for details of the method.

For high relative accuracy, using staggered PPPM allows the mesh size to be reduced by a factor of 2 in each dimension as compared to regular PPPM (for the same target accuracy). This can give up to a 4x speedup in the KSpace time (8x less mesh points, 2x more expensive). However, for low relative accuracy, the staggered PPPM mesh size may be essentially the same as for regular PPPM, which means the method will be up to 2x slower in the KSpace time (simply 2x more expensive). For more details and timings, see the *Speed tips* doc page.

Note: Using *pppm/stagger* may not give the same increase in the accuracy of energy and pressure as it does in forces, so some caution must be used if energy and/or pressure are quantities of interest, such as when using a barostat.

The *pppm/disp* and *pppm/disp/tip4p* styles add a mesh-based long-range dispersion sum option for 1/r^6 potentials *(Isele-Holder)*, similar to the *ewald/disp* style. The 1/r^6 capability means that Lennard-Jones or Buckingham potentials can be used without a cutoff, i.e. they become full long-range potentials.

For these styles, you will possibly want to adjust the default choice of parameters by using the *kspace_modify* command. This can be done by either choosing the Ewald and grid parameters, or by specifying separate accuracies for the real and kspace calculations. When not making any settings, the simulation will stop with an error message. Further information on the influence of the parameters and how to choose them is described in *(Isele-Holder)*, *(Isele-Holder2)* and the *Howto dispersion* doc page.

Note: All of the PPPM styles can be used with single-precision FFTs by using the compiler switch -DFFT_SINGLE for the FFT_INC setting in your low-level Makefile. This setting also changes some of the PPPM operations (e.g. mapping charge to mesh and interpolating electric fields to particles) to be performed in single precision. This option can speed-up long-range calculations, particularly in parallel or on GPUs. The use of the -DFFT_SINGLE flag is discussed on the *Build settings* doc page. MSM does not currently support the -DFFT_SINGLE compiler switch.

The *msm* style invokes a multi-level summation method MSM solver, *(Hardy)* or *(Hardy2)*, which maps atom charge to a 3d mesh, and uses a multi-level hierarchy of coarser and coarser meshes on which direct Coulomb solvers are done. This method does not use FFTs and scales as N. It may therefore be faster than the other K-space solvers

for relatively large problems when running on large core counts. MSM can also be used for non-periodic boundary conditions and for mixed periodic and non-periodic boundaries.

MSM is most competitive versus Ewald and PPPM when only relatively low accuracy forces, about 1e-4 relative error or less accurate, are needed. Note that use of a larger Coulombic cutoff (i.e. 15 angstroms instead of 10 angstroms) provides better MSM accuracy for both the real space and grid computed forces.

Currently calculation of the full pressure tensor in MSM is expensive. Using the *kspace_modify pressure/scalar yes* command provides a less expensive way to compute the scalar pressure (Pxx + Pyy + Pzz)/3.0. The scalar pressure can be used, for example, to run an isotropic barostat. If the full pressure tensor is needed, then calculating the pressure at every timestep or using a fixed pressure simulation with MSM will cause the code to run slower.

The *scafacos* style is a wrapper on the ScaFaCoS Coulomb solver library which provides a variety of solver methods which can be used with LAMMPS. The paper by *(Who)* gives an overview of ScaFaCoS.

ScaFaCoS was developed by a consortium of German research facilities with a BMBF (German Ministry of Science and Education) funded project in 2009-2012. Participants of the consortium were the Universities of Bonn, Chemnitz, Stuttgart, and Wuppertal as well as the Forschungszentrum Juelich.

The library is available for download at "http://scafacos.de" or can be cloned from the git-repository "git://github.com/scafacos/scafacos.git".

In order to use this KSpace style, you must download and build the ScaFaCoS library, then build LAMMPS with the USER-SCAFACOS package installed package which links LAMMPS to the ScaFaCoS library. See details on *this page*.

Note: Unlike other KSpace solvers in LAMMPS, ScaFaCoS computes all Coulombic interactions, both short- and long-range. Thus you should NOT use a Coulombic pair style when using kspace_style scafacos. This also means the total Coulombic energy (short- and long-range) will be tallied for *thermodynamic output* command as part of the *elong* keyword; the *ecoul* keyword will be zero.

Note: See the current restriction below about use of ScaFaCoS in LAMMPS with molecular charged systems or the TIP4P water model.

The specified *method* determines which ScaFaCoS algorithm is used. These are the ScaFaCoS methods currently available from LAMMPS:

- *fmm* = Fast Multi-Pole method
- *p2nfft* = FFT-based Coulomb solver
- *ewald* = Ewald summation
- *direct* = direct O(N^2) summation
- *p3m* = PPPM

We plan to support additional ScaFaCoS solvers from LAMMPS in the future. For an overview of the included solvers, refer to *(Sutmann)*

The specified *accuracy* is similar to the accuracy setting for other LAMMPS KSpace styles, but is passed to ScaFaCoS, which can interpret it in different ways for different methods it supports. Within the ScaFaCoS library the *accuracy* is treated as a tolerance level (either absolute or relative) for the chosen quantity, where the quantity can be either the Columic field values, the per-atom Columic energy or the total Columic energy. To select from these options, see the *kspace_modify scafacos accuracy* doc page.

The *kspace_modify scafacos* command also explains other ScaFaCoS options currently exposed to LAMMPS.

The specified *accuracy* determines the relative RMS error in per-atom forces calculated by the long-range solver. It is set as a dimensionless number, relative to the force that two unit point charges (e.g. 2 monovalent ions) exert on each other at a distance of 1 Angstrom. This reference value was chosen as representative of the magnitude of electrostatic forces in atomic systems. Thus an accuracy value of 1.0e-4 means that the RMS error will be a factor of 10000 smaller than the reference force.

The accuracy setting is used in conjunction with the pairwise cutoff to determine the number of K-space vectors for style *ewald* or the grid size for style *pppm* or *msm*.

Note that style *pppm* only computes the grid size at the beginning of a simulation, so if the length or triclinic tilt of the simulation cell increases dramatically during the course of the simulation, the accuracy of the simulation may degrade. Likewise, if the *kspace_modify slab* option is used with shrink-wrap boundaries in the z-dimension, and the box size changes dramatically in z. For example, for a triclinic system with all three tilt factors set to the maximum limit, the PPPM grid should be increased roughly by a factor of 1.5 in the y direction and 2.0 in the z direction as compared to the same system using a cubic orthogonal simulation cell. One way to handle this issue if you have a long simulation where the box size changes dramatically, is to break it into shorter simulations (multiple *run* commands). This works because the grid size is re-computed at the beginning of each run. Another way to ensure the described accuracy requirement is met is to run a short simulation at the maximum expected tilt or length, note the required grid size, and then use the *kspace_modify* *mesh* command to manually set the PPPM grid size to this value for the long run. The simulation then will be "too accurate" for some portion of the run.

RMS force errors in real space for *ewald* and *pppm* are estimated using equation 18 of *(Kolafa)*, which is also referenced as equation 9 of *(Petersen)*. RMS force errors in K-space for *ewald* are estimated using equation 11 of *(Petersen)*, which is similar to equation 32 of *(Kolafa)*. RMS force errors in K-space for *pppm* are estimated using equation 38 of *(Deserno)*. RMS force errors for *msm* are estimated using ideas from chapter 3 of *(Hardy)*, with equation 3.197 of particular note. When using *msm* with non-periodic boundary conditions, it is expected that the error estimation will be too pessimistic. RMS force errors for dipoles when using *ewald/disp* or *ewald/dipole* are estimated using equations 33 and 46 of *(Wang)*. The RMS force errors for *pppm/dipole* are estimated using the equations in *(Cerda)*.

See the *kspace_modify* command for additional options of the K-space solvers that can be set, including a *force* option for setting an absolute RMS error in forces, as opposed to a relative RMS error.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

More specifically, the *pppm/gpu* style performs charge assignment and force interpolation calculations on the GPU. These processes are performed either in single or double precision, depending on whether the -DFFT_SINGLE setting was specified in your low-level Makefile, as discussed above. The FFTs themselves are still calculated on the CPU. If *pppm/gpu* is used with a GPU-enabled pair style, part of the PPPM calculation can be performed concurrently on the GPU while other calculations for non-bonded and bonded force calculation are performed on the CPU.

The *pppm/kk* style performs charge assignment and force interpolation calculations, along with the FFTs themselves, on the GPU or (optionally) threaded on the CPU when using OpenMP and FFTW3.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP, and OPT packages respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

15.66.4 Restrictions

Note that the long-range electrostatic solvers in LAMMPS assume conducting metal (tinfoil) boundary conditions for both charge and dipole interactions. Vacuum boundary conditions are not currently supported.

The *ewald/disp*, *ewald*, *pppm*, and *msm* styles support non-orthogonal (triclinic symmetry) simulation boxes. However, triclinic simulation cells may not yet be supported by suffix versions of these styles.

All of the kspace styles are part of the KSPACE package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

For MSM, a simulation must be 3d and one can use any combination of periodic, non-periodic, or shrink-wrapped boundaries (specified using the *boundary* command).

For Ewald and PPPM, a simulation must be 3d and periodic in all dimensions. The only exception is if the slab option is set with *kspace_modify*, in which case the xy dimensions must be periodic and the z dimension must be non-periodic.

The scafacos KSpace style will only be enabled if LAMMPS is built with the USER-SCAFACOS package. See the *Build package* doc page for more info.

The use of ScaFaCos in LAMMPS does not yet support molecular charged systems where the short-range Coulombic interactions between atoms in the same bond/angle/dihedral are weighted by the *special_bonds* command. Likewise it does not support the "TIP4P water style" where a fictitious charge site is introduced in each water molecule. Finally, the methods *p3m* and *ewald* do not support computing the virial, so this contribution is not included.

15.66.5 Related commands

kspace_modify, *pair_style lj/cut/coul/long*, *pair_style lj/charmm/coul/long*, *pair_style lj/long/coul/long*, *pair_style buck/coul/long*

15.66.6 Default

```
kspace_style none
```

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15.67 label command

15.67.1 Syntax

```
label ID
```

- ID = string used as label name

15.67.2 Examples

```
label xyz
label loop
```

15.67.3 Description

Label this line of the input script with the chosen ID. Unless a jump command was used previously, this does nothing. But if a *jump* command was used with a label argument to begin invoking this script file, then all command lines in the script prior to this line will be ignored. I.e. execution of the script will begin at this line. This is useful for looping over a section of the input script as discussed in the *jump* command.

15.67.4 Restrictions

none

Related commands: none

Default: none

15.68 lattice command

15.68.1 Syntax

```
lattice style scale keyword values ...
```

- style = *none* or *sc* or *bcc* or *fcc* or *hcp* or *diamond* or *sq* or *sq2* or *hex* or *custom*
- scale = scale factor between lattice and simulation box

```
scale = reduced density rho* (for LJ units)
scale = lattice constant in distance units (for all other units)
```

- zero or more keyword/value pairs may be appended
- keyword = *origin* or *orient* or *spacing* or *a1* or *a2* or *a3* or *basis*

```
origin values = x y z
  x,y,z = fractions of a unit cell (0 <= x,y,z < 1)
orient values = dim i j k
  dim = x or y or z
  i,j,k = integer lattice directions
spacing values = dx dy dz
  dx,dy,dz = lattice spacings in the x,y,z box directions
a1,a2,a3 values = x y z
  x,y,z = primitive vector components that define unit cell
basis values = x y z
  x,y,z = fractional coords of a basis atom (0 <= x,y,z < 1)
```

15.68.2 Examples

```
lattice fcc 3.52
lattice hex 0.85
lattice sq 0.8 origin 0.0 0.5 0.0 orient x 1 1 0 orient y -1 1 0
lattice custom 3.52 a1 1.0 0.0 0.0 a2 0.5 1.0 0.0 a3 0.0 0.0 0.5 &
                    basis 0.0 0.0 0.0 basis 0.5 0.5 0.5
lattice none 2.0
```

15.68.3 Description

Define a lattice for use by other commands. In LAMMPS, a lattice is simply a set of points in space, determined by a unit cell with basis atoms, that is replicated infinitely in all dimensions. The arguments of the lattice command can be used to define a wide variety of crystallographic lattices.

A lattice is used by LAMMPS in two ways. First, the *create_atoms* command creates atoms on the lattice points inside the simulation box. Note that the *create_atoms* command allows different atom types to be assigned to different basis atoms of the lattice. Second, the lattice spacing in the x,y,z dimensions implied by the lattice, can be used by other commands as distance units (e.g. *create_box*, *region* and *velocity*), which are often convenient to use when the underlying problem geometry is atoms on a lattice.

The lattice style must be consistent with the dimension of the simulation - see the *dimension* command. Styles *sc* or *bcc* or *fcc* or *hcp* or *diamond* are for 3d problems. Styles *sq* or *sq2* or *hex* are for 2d problems. Style *custom* can be used for either 2d or 3d problems.

A lattice consists of a unit cell, a set of basis atoms within that cell, and a set of transformation parameters (scale, origin, orient) that map the unit cell into the simulation box. The vectors a1,a2,a3 are the edge vectors of the unit cell. This is the nomenclature for "primitive" vectors in solid-state crystallography, but in LAMMPS the unit cell they determine does not have to be a "primitive cell" of minimum volume.

Note that the lattice command can be used multiple times in an input script. Each time it is invoked, the lattice attributes are re-defined and are used for all subsequent commands (that use lattice attributes). For example, a sequence of lattice, *region*, and *create_atoms* commands can be repeated multiple times to build a poly-crystalline model with different geometric regions populated with atoms in different lattice orientations.

A lattice of style *none* does not define a unit cell and basis set, so it cannot be used with the *create_atoms* command. However it does define a lattice spacing via the specified scale parameter. As explained above the lattice spacings in x,y,z can be used by other commands as distance units. No additional keyword/value pairs can be specified for the *none* style. By default, a "lattice none 1.0" is defined, which means the lattice spacing is the same as one distance unit, as defined by the *units* command.

Lattices of style *sc*, *fcc*, *bcc*, and *diamond* are 3d lattices that define a cubic unit cell with edge length = 1.0. This means a1 = 1 0 0, a2 = 0 1 0, and a3 = 0 0 1. Style *hcp* has a1 = 1 0 0, a2 = 0 sqrt(3) 0, and a3 = 0 0 sqrt(8/3). The placement of the basis atoms within the unit cell are described in any solid-state physics text. A *sc* lattice has 1 basis atom at the lower-left-bottom corner of the cube. A *bcc* lattice has 2 basis atoms, one at the corner and one at the center of the cube. A *fcc* lattice has 4 basis atoms, one at the corner and 3 at the cube face centers. A *hcp* lattice has 4 basis atoms, two in the z = 0 plane and 2 in the z = 0.5 plane. A *diamond* lattice has 8 basis atoms.

Lattices of style *sq* and *sq2* are 2d lattices that define a square unit cell with edge length = 1.0. This means a1 = 1 0 0 and a2 = 0 1 0. A *sq* lattice has 1 basis atom at the lower-left corner of the square. A *sq2* lattice has 2 basis atoms, one at the corner and one at the center of the square. A *hex* style is also a 2d lattice, but the unit cell is rectangular, with a1 = 1 0 0 and a2 = 0 sqrt(3) 0. It has 2 basis atoms, one at the corner and one at the center of the rectangle.

A lattice of style *custom* allows you to specify a1, a2, a3, and a list of basis atoms to put in the unit cell. By default, a1 and a2 and a3 are 3 orthogonal unit vectors (edges of a unit cube). But you can specify them to be of any length and non-orthogonal to each other, so that they describe a tilted parallelepiped. Via the *basis* keyword you add atoms, one at a time, to the unit cell. Its arguments are fractional coordinates (0.0 <= x,y,z < 1.0). The position vector x of a basis atom within the unit cell is thus a linear combination of the unit cell's 3 edge vectors, i.e. x = bx a1 + by a2 + bz a3, where bx,by,bz are the 3 values specified for the *basis* keyword.

This sub-section discusses the arguments that determine how the idealized unit cell is transformed into a lattice of points within the simulation box.

The *scale* argument determines how the size of the unit cell will be scaled when mapping it into the simulation box. I.e. it determines a multiplicative factor to apply to the unit cell, to convert it to a lattice of the desired size and distance units in the simulation box. The meaning of the *scale* argument depends on the *units* being used in your simulation.

For all unit styles except *lj*, the scale argument is specified in the distance units defined by the unit style. For example, in *real* or *metal* units, if the unit cell is a unit cube with edge length 1.0, specifying scale = 3.52 would create a cubic lattice with a spacing of 3.52 Angstroms. In *cgs* units, the spacing would be 3.52 cm.

For unit style *lj*, the scale argument is the Lennard-Jones reduced density, typically written as rho*. LAMMPS converts this value into the multiplicative factor via the formula "factor^dim = rho/rho*", where rho = N/V with V = the volume of the lattice unit cell and N = the number of basis atoms in the unit cell (described below), and dim = 2 or 3 for the dimensionality of the simulation. Effectively, this means that if LJ particles of size sigma = 1.0 are used in the simulation, the lattice of particles will be at the desired reduced density.

The *origin* option specifies how the unit cell will be shifted or translated when mapping it into the simulation box. The x,y,z values are fractional values (0.0 <= x,y,z < 1.0) meaning shift the lattice by a fraction of the lattice spacing in each dimension. The meaning of "lattice spacing" is discussed below.

The *orient* option specifies how the unit cell will be rotated when mapping it into the simulation box. The *dim* argument is one of the 3 coordinate axes in the simulation box. The other 3 arguments are the crystallographic direction in the lattice that you want to orient along that axis, specified as integers. E.g. "orient x 2 1 0" means the x-axis in the simulation box will be the [210] lattice direction, and similarly for y and z. The 3 lattice directions you specify do not have to be unit vectors, but they must be mutually orthogonal and obey the right-hand rule, i.e. (X cross Y) points in the Z direction.

Note: The preceding paragraph describing lattice directions is only valid for orthogonal cubic unit cells (or square in 2d). If you are using a *hcp* or *hex* lattice or the more general lattice style *custom* with non-orthogonal a1,a2,a3 vectors,

then you should think of the 3 *orient* vectors as creating a 3x3 rotation matrix which is applied to a1,a2,a3 to rotate the original unit cell to a new orientation in the simulation box.

Several LAMMPS commands have the option to use distance units that are inferred from "lattice spacings" in the x,y,z box directions. E.g. the *region* command can create a block of size 10x20x20, where 10 means 10 lattice spacings in the x direction.

Note: Though they are called lattice spacings, all the commands that have a "units lattice" option, simply use the 3 values as scale factors on the distance units defined by the *units* command. Thus if you do not like the lattice spacings computed by LAMMPS (e.g. for a non-orthogonal or rotated unit cell), you can define the 3 values to be whatever you wish, via the *spacing* option.

If the *spacing* option is not specified, the lattice spacings are computed by LAMMPS in the following way. A unit cell of the lattice is mapped into the simulation box (scaled and rotated), so that it now has (perhaps) a modified size and orientation. The lattice spacing in X is defined as the difference between the min/max extent of the x coordinates of the 8 corner points of the modified unit cell (4 in 2d). Similarly, the Y and Z lattice spacings are defined as the difference in the min/max of the y and z coordinates.

Note that if the unit cell is orthogonal with axis-aligned edges (no rotation via the *orient* keyword), then the lattice spacings in each dimension are simply the scale factor (described above) multiplied by the length of a1,a2,a3. Thus a *hex* style lattice with a scale factor of 3.0 Angstroms, would have a lattice spacing of 3.0 in x and 3*sqrt(3.0) in y.

Note: For non-orthogonal unit cells and/or when a rotation is applied via the *orient* keyword, then the lattice spacings computed by LAMMPS are typically less intuitive. In particular, in these cases, there is no guarantee that a particular lattice spacing is an integer multiple of the periodicity of the lattice in that direction. Thus, if you create an orthogonal periodic simulation box whose size in a dimension is a multiple of the lattice spacing, and then fill it with atoms via the *create_atoms* command, you will NOT necessarily create a periodic system. I.e. atoms may overlap incorrectly at the faces of the simulation box.

The *spacing* option sets the 3 lattice spacings directly. All must be non-zero (use 1.0 for dz in a 2d simulation). The specified values are multiplied by the multiplicative factor described above that is associated with the scale factor. Thus a spacing of 1.0 means one unit cell edge length independent of the scale factor. As mentioned above, this option can be useful if the spacings LAMMPS computes are inconvenient to use in subsequent commands, which can be the case for non-orthogonal or rotated lattices.

Note that whenever the lattice command is used, the values of the lattice spacings LAMMPS calculates are printed out. Thus their effect in commands that use the spacings should be decipherable.

Example commands for generating a Wurtzite crystal (courtesy of Aidan Thompson), with its 8 atom unit cell.

```
variable a equal  4.340330
variable b equal  $a*sqrt(3.0)
variable c equal  $a*sqrt(8.0/3.0)

variable 1_3 equal 1.0/3.0
variable 2_3 equal 2.0/3.0
variable 1_6 equal 1.0/6.0
variable 5_6 equal 5.0/6.0
variable 1_12 equal 1.0/12.0
variable 5_12 equal 5.0/12.0
```

```
lattice custom    1.0     &
        a1      $a      0.0     0.0     &
        a2      0.0     $b      0.0     &
        a3      0.0     0.0     $c      &
        basis   0.0     0.0     0.0     &
        basis   0.5     0.5     0.0     &
        basis   ${1_3}  0.0     0.5     &
        basis   ${5_6}  0.5     0.5     &
        basis   0.0     0.0     0.625   &
        basis   0.5     0.5     0.625   &
        basis   ${1_3}  0.0     0.125   &
        basis   ${5_6}  0.5     0.125

region myreg block 0 1 0 1 0 1
create_box      2 myreg
create_atoms    1 box      &
        basis   5       2       &
        basis   6       2       &
        basis   7       2       &
        basis   8       2
```

15.68.4 Restrictions

The *a1,a2,a3,basis* keywords can only be used with style *custom*.

15.68.5 Related commands

dimension, *create_atoms*, *region*

15.68.6 Default

```
lattice none 1.0
```

For other lattice styles, the option defaults are origin = 0.0 0.0 0.0, orient = x 1 0 0, orient = y 0 1 0, orient = z 0 0 1, a1 = 1 0 0, a2 = 0 1 0, and a3 = 0 0 1.

15.69 log command

15.69.1 Syntax

```
log file keyword
```

- file = name of new logfile
- keyword = *append* if output should be appended to logfile (optional)

15.69.2 Examples

```
log log.equil
log log.equil append
```

15.69.3 Description

This command closes the current LAMMPS log file, opens a new file with the specified name, and begins logging information to it. If the specified file name is *none*, then no new log file is opened. If the optional keyword *append* is specified, then output will be appended to an existing log file, instead of overwriting it.

If multiple processor partitions are being used, the file name should be a variable, so that different processors do not attempt to write to the same log file.

The file "log.lammps" is the default log file for a LAMMPS run. The name of the initial log file can also be set by the *-log command-line switch*.

15.69.4 Restrictions

none

Related commands: none

15.69.5 Default

The default LAMMPS log file is named log.lammps

15.70 mass command

15.70.1 Syntax

```
mass I value
```

- I = atom type (see asterisk form below)
- value = mass

15.70.2 Examples

```
mass 1 1.0
mass * 62.5
mass 2* 62.5
```

15.70.3 Description

Set the mass for all atoms of one or more atom types. Per-type mass values can also be set in the *read_data* data file using the "Masses" keyword. See the *units* command for what mass units to use.

The I index can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to set the mass for multiple atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

A line in a *data file* that follows the "Masses" keyword specifies mass using the same format as the arguments of the mass command in an input script, except that no wild-card asterisk can be used. For example, under the "Masses" section of a data file, the line that corresponds to the 1st example above would be listed as

```
1 1.0
```

Note that the mass command can only be used if the *atom style* requires per-type atom mass to be set. Currently, all but the *sphere* and *ellipsoid* and *peri* styles do. They require mass to be set for individual particles, not types. Per-atom masses are defined in the data file read by the *read_data* command, or set to default values by the *create_atoms* command. Per-atom masses can also be set to new values by the *set mass* or *set density* commands.

Also note that *pair_style eam* and *pair_style bop* commands define the masses of atom types in their respective potential files, in which case the mass command is normally not used.

If you define a *hybrid atom style* which includes one (or more) sub-styles which require per-type mass and one (or more) sub-styles which require per-atom mass, then you must define both. However, in this case the per-type mass will be ignored; only the per-atom mass will be used by LAMMPS.

15.70.4 Restrictions

This command must come after the simulation box is defined by a *read_data*, *read_restart*, or *create_box* command.

All masses must be defined before a simulation is run. They must also all be defined before a *velocity* or *fix shake* command is used.

The mass assigned to any type or atom must be > 0.0.

Related commands: none

Default: none

15.71 message command

15.71.1 Syntax

```
message which protocol mode arg
```

- which = *client* or *server* or *quit*
- protocol = *md* or *mc*
- mode = *file* or *zmq* or *mpi/one* or *mpi/two*

```
file arg = filename
  filename = file used for message exchanges
zmq arg = socket-ID
```

```
      socket-ID for client = localhost:5555, see description below
      socket-ID for server = *:5555, see description below
    mpi/one arg = none
    mpi/two arg = filename
      filename = file used to establish communication between 2 MPI jobs
```

15.71.2 Examples

```
message client md file tmp.couple
message server md file tmp.couple

message client md zmq localhost:5555
message server md zmq *:5555

message client md mpi/one
message server md mpi/one

message client md mpi/two tmp.couple
message server md mpi/two tmp.couple

message quit
```

15.71.3 Description

Establish a messaging protocol between LAMMPS and another code for the purpose of client/server coupling.

The *Howto client/server* doc page gives an overview of client/server coupling of LAMMPS with another code where one code is the "client" and sends request messages to a "server" code. The server responds to each request with a reply message. This enables the two codes to work in tandem to perform a simulation.

The *which* argument defines LAMMPS to be the client or the server.

As explained below the *quit* option should be used when LAMMPS is finished as a client. It sends a message to the server to tell it to shut down.

The *protocol* argument defines the format and content of messages that will be exchanged between the two codes. The current options are:

- md = run dynamics with another code
- mc = perform Monte Carlo moves with another code

For protocol *md*, LAMMPS can be either a client or server. See the *server md* doc page for details on the protocol.

For protocol *mc*, LAMMPS can be the server. See the *server mc* doc page for details on the protocol.

The *mode* argument specifies how messages are exchanged between the client and server codes. Both codes must use the same mode and use consistent parameters.

For mode *file*, the 2 codes communicate via binary files. They must use the same filename, which is actually a file prefix. Several files with that prefix will be created and deleted as a simulation runs. The filename can include a path. Both codes must be able to access the path/file in a common filesystem.

For mode *zmq*, the 2 codes communicate via a socket on the server code's machine. Support for socket messaging is provided by the open-source ZeroMQ library, which must be installed on your system. The client specifies an IP address (IPv4 format) or the DNS name of the machine the server code is running on, followed by a 4-digit port ID for the socket, separated by a colon. E.g.

```
localhost:5555        # client and server running on same machine
192.168.1.1:5555      # server is 192.168.1.1
deptbox.uni.edu:5555  # server is deptbox.uni.edu
```

The server specifies "*:5555" where "*" represents all available interfaces on the server's machine, and the port ID must match what the client specifies.

Note: What are allowed port IDs?

Note: Additional explanation is needed here about how to use the *zmq* mode on a parallel machine, e.g. a cluster with many nodes.

For mode *mpi/one*, the 2 codes communicate via MPI and are launched by the same mpirun command, e.g. with this syntax for OpenMPI:

```
mpirun -np 2 lmp_mpi -mpicolor 0 -in in.client -log log.client : -np 4 othercode args␣
↪ # LAMMPS is client
mpirun -np 2 othercode args : -np 4 lmp_mpi -mpicolor 1 -in in.server  # LAMMPS is␣
↪server
```

Note the use of the "-mpicolor color" command-line argument with LAMMPS. See the *command-line args* doc page for further explanation.

For mode *mpi/two*, the 2 codes communicate via MPI, but are launched be 2 separate mpirun commands. The specified *filename* argument is a file the 2 MPI processes will use to exchange info so that an MPI inter-communicator can be established to enable the 2 codes to send MPI messages to each other. Both codes must be able to access the path/file in a common filesystem.

Normally, the message client or message server command should be used at the top of a LAMMPS input script. It performs an initial handshake with the other code to setup messaging and to verify that both codes are using the same message protocol and mode. Assuming both codes are launched at (nearly) the same time, the other code should perform the same kind of initialization.

If LAMMPS is the client code, it will begin sending messages when a LAMMPS client command begins its operation. E.g. for the *fix client/md* command, it is when a *run* command is executed.

If LAMMPS is the server code, it will begin receiving messages when the *server* command is invoked.

If LAMMPS is being used as a client, the message quit command will terminate its messaging with the server. If you do not use this command and just allow LAMMPS to exit, then the server will continue to wait for further messages. This may not be a problem, but if both the client and server programs were launched in the same batch script, then if the server runs indefinitely, it may consume the full allocation of computer time, even if the calculation finishes sooner.

Note that if LAMMPS is the client or server, it will continue processing the rest of its input script after client/server communication terminates.

If both codes cooperate in this manner, a new round of client/server messaging can be initiated after termination by re-using a 2nd message command in your LAMMPS input script, followed by a new fix client or server command, followed by another message quit command (if LAMMPS is the client). As an example, this can be performed in

a loop to use a quantum code as a server to compute quantum forces for multiple LAMMPS data files or periodic snapshots while running dynamics.

15.71.4 Restrictions

This command is part of the MESSAGE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

15.71.5 Related commands

server, *fix client/md*

Default: none

15.72 min_modify command

15.72.1 Syntax

```
min_modify keyword values ...
```

- one or more keyword/value pairs may be listed

```
keyword = dmax or line or norm or alpha_damp or discrete_factor or␣
↪integrator or tmax
  dmax value = max
    max = maximum distance for line search to move (distance units)
  line value = backtrack or quadratic or forcezero or spin_cubic or spin_
↪none
    backtrack,quadratic,forcezero,spin_cubic,spin_none = style of␣
↪linesearch to use
  norm value = two or max
    two = Euclidean two-norm (length of 3N vector)
    inf = max force component across all 3-vectors
    max = max force norm across all 3-vectors
  alpha_damp value = damping
    damping = fictitious Gilbert damping for spin minimization (adim)
  discrete_factor value = factor
    factor = discretization factor for adaptive spin timestep (adim)
  integrator value = eulerimplicit or verlet
    time integration scheme for fire minimization
  tmax value = factor
    factor = maximum adaptive timestep for fire minimization (adim)
```

15.72.2 Examples

```
min_modify dmax 0.2
min_modify integrator verlet tmax 4
```

15.72.3 Description

This command sets parameters that affect the energy minimization algorithms selected by the *min_style* command. The various settings may affect the convergence rate and overall number of force evaluations required by a minimization, so users can experiment with these parameters to tune their minimizations.

The *cg* and *sd* minimization styles have an outer iteration and an inner iteration which is steps along a one-dimensional line search in a particular search direction. The *dmax* parameter is how far any atom can move in a single line search in any dimension (x, y, or z). For the *quickmin* and *fire* minimization styles, the *dmax* setting is how far any atom can move in a single iteration (timestep). Thus a value of 0.1 in real *units* means no atom will move further than 0.1 Angstroms in a single outer iteration. This prevents highly overlapped atoms from being moved long distances (e.g. through another atom) due to large forces.

The choice of line search algorithm for the *cg* and *sd* minimization styles can be selected via the *line* keyword. The default *quadratic* line search algorithm starts out using the robust backtracking method described below. However, once the system gets close to a local minimum and the linesearch steps get small, so that the energy is approximately quadratic in the step length, it uses the estimated location of zero gradient as the linesearch step, provided the energy change is downhill. This becomes more efficient than backtracking for highly-converged relaxations. The *forcezero* line search algorithm is similar to *quadratic*. It may be more efficient than *quadratic* on some systems.

The backtracking search is robust and should always find a local energy minimum. However, it will "converge" when it can no longer reduce the energy of the system. Individual atom forces may still be larger than desired at this point, because the energy change is measured as the difference of two large values (energy before and energy after) and that difference may be smaller than machine epsilon even if atoms could move in the gradient direction to reduce forces further.

The choice of a norm can be modified for the min styles *cg*, *sd*, *quickmin*, *fire*, *fire/old*, *spin*, *spin/cg* and *spin/lbfgs* using the *norm* keyword. The default *two* norm computes the 2-norm (Euclidean length) of the global force vector:

$$||\vec{F}||_2 = \sqrt{\vec{F}_1 + \cdots + \vec{F}_N}$$

The *max* norm computes the length of the 3-vector force for each atom (2-norm), and takes the maximum value of those across all atoms

$$||\vec{F}||_{max} = \max\left(||\vec{F}_1||, \cdots, ||\vec{F}_N||\right)$$

The *inf* norm takes the maximum component across the forces of all atoms in the system:

$$||\vec{F}||_{inf} = \max\left(|F_1^1|, |F_1^2|, |F_1^3| \cdots, |F_N^1|, |F_N^2|, |F_N^3|\right)$$

For the min styles *spin*, *spin/cg* and *spin/lbfgs*, the force norm is replaced by the spin-torque norm.

Keywords *alpha_damp* and *discrete_factor* only make sense when a *min_spin* command is declared. Keyword *alpha_damp* defines an analog of a magnetic Gilbert damping. It defines a relaxation rate toward an equilibrium for a given magnetic system. Keyword *discrete_factor* defines a discretization factor for the adaptive timestep used in the *spin* minimization. See *min_spin* for more information about those quantities.

The choice of a line search algorithm for the *spin/cg* and *spin/lbfgs* styles can be specified via the *line* keyword. The *spin_cubic* and *spin_none* keywords only make sense when one of those two minimization styles is declared. The *spin_cubic* performs the line search based on a cubic interpolation of the energy along the search direction. The

spin_none keyword deactivates the line search procedure. The *spin_none* is a default value for *line* keyword for both *spin/lbfgs* and *spin/cg*. Convergence of *spin/lbfgs* can be more robust if *spin_cubic* line search is used.

The Newton *integrator* used for *fire* minimization can be selected to be either the symplectic Euler (*eulerimplicit*) or velocity Verlet (*verlet*). *tmax* defines the maximum value for the adaptive timestep during a *fire* minimization. It is a multiplication factor applied to the current *timestep* (not in time unit). For example, *tmax* = 4.0 with a *timestep* of 2fs, means that the maximum value the timestep can reach during a *fire* minimization is 4fs. Note that parameter defaults has been chosen to be reliable in most cases, but one should consider adjusting *timestep* and *tmax* to optimize the minimization for large or complex systems. Other parameters of the *fire* minimization can be tuned (*tmin*, *delaystep*, *dtgrow*, *dtshrink*, *alpha0*, and *alphashrink*). Please refer to the references describing the *min_style fire*. An additional stopping criteria *vdfmax* is used by *fire* in order to avoid unnecessary looping when it is reasonable to think the system will not be relaxed further. Note that in this case the system will NOT have reached your minimization criteria. This could happen when the system comes to be stuck in a local basin of the phase space. *vdfmax* is the maximum number of consecutive iterations with P(t) < 0.

The *min_style fire* is an optimized implementation of *min_style fire/old*. It can however behave similarly to the *fire/old* style by using the following set of parameters:

```
min_modify integrator eulerexplicit tmax 10.0 tmin 0.0 delaystep 5 &
          dtgrow 1.1 dtshrink 0.5 alpha0 0.1 alphashrink 0.99 &
          vdfmax 100000 halfstepback no initialdelay no
```

15.72.4 Restrictions

For magnetic GNEB calculations, only *spin_none* value for *line* keyword can be used when minimization styles *spin/cg* and *spin/lbfgs* are employed. See *neb/spin* for more explanation.

15.72.5 Related commands

min_style, *minimize*

15.72.6 Default

The option defaults are dmax = 0.1, line = quadratic and norm = two.

For the *spin*, *spin/cg* and *spin/lbfgs* styles, the option defaults are alpha_damp = 1.0, discrete_factor = 10.0, line = spin_none, and norm = euclidean.

For the *fire* style, the option defaults are integrator = eulerimplicit, tmax = 10.0, tmin = 0.02, delaystep = 20, dtgrow = 1.1, dtshrink = 0.5, alpha0 = 0.25, alphashrink = 0.99, vdfmax = 2000, halfstepback = yes and initialdelay = yes.

15.73 min_style spin command

15.74 min_style spin/cg command

15.75 min_style spin/lbfgs command

15.75.1 Syntax

```
min_style spin
min_style spin/cg
min_style spin/lbfgs
```

15.75.2 Examples

```
min_style  spin/lbfgs
min_modify line spin_cubic discrete_factor 10.0
```

15.75.3 Description

Apply a minimization algorithm to use when a *minimize* command is performed.

Style *spin* defines a damped spin dynamics with an adaptive timestep, according to:

$$\frac{d\vec{s}_i}{dt} = \lambda\, \vec{s}_i \times (\vec{\omega}_i \times \vec{s}_i)$$

with λ a damping coefficient (similar to a Gilbert damping). λ can be defined by setting the *alpha_damp* keyword with the *min_modify* command.

The minimization procedure solves this equation using an adaptive timestep. The value of this timestep is defined by the largest precession frequency that has to be solved in the system:

$$\Delta t_{\max} = \frac{2\pi}{\kappa\, |\vec{\omega}_{\max}|}$$

with $|\vec{\omega}_{\max}|$ the norm of the largest precession frequency in the system (across all processes, and across all replicas if a spin/neb calculation is performed).

κ defines a discretization factor *discrete_factor* for the definition of this timestep. *discrete_factor* can be defined with the *min_modify* command.

Style *spin/cg* defines an orthogonal spin optimization (OSO) combined to a conjugate gradient (CG) algorithm. The *min_modify* command can be used to couple the *spin/cg* to a line search procedure, and to modify the discretization factor *discrete_factor*. By default, style *spin/cg* does not employ the line search procedure and uses the adaptive time-step technique in the same way as style *spin*.

Style *spin/lbfgs* defines an orthogonal spin optimization (OSO) combined to a limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) algorithm. By default, style *spin/lbfgs* does not employ line search procedure. If the line search procedure is not used then the discrete factor defines the maximum root mean squared rotation angle of spins by equation *pi/(5*Kappa)*. The default value for Kappa is 10. The *spin_cubic* line search option can improve the convergence of the *spin/lbfgs* algorithm.

The *min_modify* command can be used to activate the line search procedure, and to modify the discretization factor *discrete_factor*.

For more information about styles *spin/cg* and *spin/lbfgs*, see their implementation reported in *(Ivanov)*.

Note: All the *spin* styles replace the force tolerance by a torque tolerance. See *minimize* for more explanation.

Note: The *spin/cg* and *spin/lbfgs* styles can be used for magnetic NEB calculations only if the line search procedure is deactivated. See *neb/spin* for more explanation.

15.75.4 Restrictions

This minimization procedure is only applied to spin degrees of freedom for a frozen lattice configuration.

15.75.5 Related commands

min_style, *minimize*, *min_modify*

15.75.6 Default

The option defaults are *alpha_damp* = 1.0, *discrete_factor* = 10.0, *line* = spin_none and *norm* = euclidean.

(Ivanov) Ivanov, Uzdin, Jonsson. arXiv preprint arXiv:1904.02669, (2019).

15.76 min_style command

15.76.1 Syntax

```
min_style style
```

- style = *cg* or *hftn* or *sd* or *quickmin* or *fire* or *fire/old* or *spin* or *spin/cg* or *spin/lbfgs*

15.76.2 Examples

```
min_style cg
min_style spin
min_style fire
```

15.76.3 Description

Choose a minimization algorithm to use when a *minimize* command is performed.

Style *cg* is the Polak-Ribiere version of the conjugate gradient (CG) algorithm. At each iteration the force gradient is combined with the previous iteration information to compute a new search direction perpendicular (conjugate) to the previous search direction. The PR variant affects how the direction is chosen and how the CG method is restarted when it ceases to make progress. The PR variant is thought to be the most effective CG choice for most problems.

Style *hftn* is a Hessian-free truncated Newton algorithm. At each iteration a quadratic model of the energy potential is solved by a conjugate gradient inner iteration. The Hessian (second derivatives) of the energy is not formed directly, but approximated in each conjugate search direction by a finite difference directional derivative. When close to an energy minimum, the algorithm behaves like a Newton method and exhibits a quadratic convergence rate to high accuracy. In most cases the behavior of *hftn* is similar to *cg*, but it offers an alternative if *cg* seems to perform poorly. This style is not affected by the *min_modify* command.

Style *sd* is a steepest descent algorithm. At each iteration, the search direction is set to the downhill direction corresponding to the force vector (negative gradient of energy). Typically, steepest descent will not converge as quickly as CG, but may be more robust in some situations.

Style *quickmin* is a damped dynamics method described in *(Sheppard)*, where the damping parameter is related to the projection of the velocity vector along the current force vector for each atom. The velocity of each atom is initialized to 0.0 by this style, at the beginning of a minimization.

Style *fire* is a damped dynamics method described in *(Bitzek)*, which is similar to *quickmin* but adds a variable timestep and alters the projection operation to maintain components of the velocity non-parallel to the current force vector. The velocity of each atom is initialized to 0.0 by this style, at the beginning of a minimization. This style correspond to an optimized version described in *(Guenole)* that include different time integration schemes and defaults parameters. The default parameters can be modified with the command *min_modify*.

Style *fire/old* is the original implementation of *fire* in Lammps, conserved for backward compatibility. The main differences regarding the current version *fire* are: time integration by Explicit Euler only, different sequence in maintaining velocity components non-parallel to the current force vector and hard-coded minimization parameters. A complete description of the differences between *fire/old* and *fire* can be found in *(Guenole)* (where the current *fire* in LAMMPS is called *fire2.0*). By using an appropriate set of parameters, *fire* can behave similar to *fire/old*, as described in the *min_modify* command.

Style *spin* is a damped spin dynamics with an adaptive timestep.

Style *spin/cg* uses an orthogonal spin optimization (OSO) combined to a conjugate gradient (CG) approach to minimize spin configurations.

Style *spin/lbfgs* uses an orthogonal spin optimization (OSO) combined to a limited-memory Broyden-Fletcher-Goldfarb-Shanno (LBFGS) approach to minimize spin configurations.

See the *min/spin* doc page for more information about the *spin*, *spin/cg* and *spin/lbfgs* styles.

Either the *quickmin*, *fire* and *fire/old* styles are useful in the context of nudged elastic band (NEB) calculations via the *neb* command.

Either the *spin*, *spin/cg* and *spin/lbfgs* styles are useful in the context of magnetic geodesic nudged elastic band (GNEB) calculations via the *neb/spin* command.

Note: The damped dynamic minimizers use whatever timestep you have defined via the *timestep* command. Often they will converge more quickly if you use a timestep about 10x larger than you would normally use for dynamics simulations. For *fire*, the default timestep is recommended to be equal to the one you would normally use for dynamics simulations.

Note: The *quickmin*, *fire*, *fire/old*, *hftn*, and *cg/kk* styles do not yet support the use of the *fix box/relax* command or minimizations involving the electron radius in *eFF* models.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

15.76.4 Restrictions

none

15.76.5 Related commands

min_modify, *minimize*, *neb*

15.76.6 Default

```
min_style cg
```

(Sheppard) Sheppard, Terrell, Henkelman, J Chem Phys, 128, 134106 (2008). See ref 1 in this paper for original reference to Qmin in Jonsson, Mills, Jacobsen.

(Bitzek) Bitzek, Koskinen, Gahler, Moseler, Gumbsch, Phys Rev Lett, 97, 170201 (2006).

(Guenole) Guenole, Noehring, Vaid, Houlle, Xie, Prakash, Bitzek, Comput Mater Sci, (2020), in press (arXiv:190802038).

15.77 minimize command

15.78 minimize/kk command

15.78.1 Syntax

```
minimize etol ftol maxiter maxeval
```

- etol = stopping tolerance for energy (unitless)
- ftol = stopping tolerance for force (force units)
- maxiter = max iterations of minimizer
- maxeval = max number of force/energy evaluations

15.78.2 Examples

```
minimize 1.0e-4 1.0e-6 100 1000
minimize 0.0 1.0e-8 1000 100000
```

15.78.3 Description

Perform an energy minimization of the system, by iteratively adjusting atom coordinates. Iterations are terminated when one of the stopping criteria is satisfied. At that point the configuration will hopefully be in local potential energy minimum. More precisely, the configuration should approximate a critical point for the objective function (see below), which may or may not be a local minimum.

The minimization algorithm used is set by the *min_style* command. Other options are set by the *min_modify* command. Minimize commands can be interspersed with *run* commands to alternate between relaxation and dynamics. The minimizers bound the distance atoms move in one iteration, so that you can relax systems with highly overlapped atoms (large energies and forces) by pushing the atoms off of each other.

Alternate means of relaxing a system are to run dynamics with a small or *limited timestep*. Or dynamics can be run using *fix viscous* to impose a damping force that slowly drains all kinetic energy from the system. The *pair_style soft* potential can be used to un-overlap atoms while running dynamics. un-overlap atoms while running dynamics.

Note that you can minimize some atoms in the system while holding the coordinates of other atoms fixed by applying *fix setforce* to the other atoms. See a fuller discussion of using fixes while minimizing below.

The *minimization styles* *cg*, *sd*, and *hftn* involves an outer iteration loop which sets the search direction along which atom coordinates are changed. An inner iteration is then performed using a line search algorithm. The line search typically evaluates forces and energies several times to set new coordinates. Currently, a backtracking algorithm is used which may not be optimal in terms of the number of force evaluations performed, but appears to be more robust than previous line searches we've tried. The backtracking method is described in Nocedal and Wright's Numerical Optimization (Procedure 3.1 on p 41).

The *minimization styles* *quickmin*, *fire* and *fire/old* perform damped dynamics using an Euler integration step. Thus they require a *timestep* be defined.

Note: The damped dynamic minimizers use whatever timestep you have defined via the *timestep* command. Often they will converge more quickly if you use a timestep about 10x larger than you would normally use for dynamics simulations.

In all cases, the objective function being minimized is the total potential energy of the system as a function of the N atom coordinates:

$$E(r_1, r_2, \ldots, r_N) = \sum_{i,j} E_{pair}(r_i, r_j) + \sum_{ij} E_{bond}(r_i, r_j) + \sum_{ijk} E_{angle}(r_i, r_j, r_k) + \sum_{ijkl} E_{dihedral}(r_i, r_j, r_k, r_l) + \sum_{ijkl} E_{improper}(r_i, r_j, r_k, r_l) + \sum_{i} E_{fix}(r_i)$$

where the first term is the sum of all non-bonded *pairwise interactions* including *long-range Coulombic interactions*, the 2nd through 5th terms are *bond*, *angle*, *dihedral*, and *improper* interactions respectively, and the last term is energy due to *fixes* which can act as constraints or apply force to atoms, such as through interaction with a wall. See the discussion below about how fix commands affect minimization.

The starting point for the minimization is the current configuration of the atoms.

The minimization procedure stops if any of several criteria are met:

- the change in energy between outer iterations is less than *etol*
- the 2-norm (length) of the global force vector is less than the *ftol*
- the line search fails because the step distance backtracks to 0.0
- the number of outer iterations or timesteps exceeds *maxiter*
- the number of total force evaluations exceeds *maxeval*

Note: the *minimization style* *spin*, *spin/cg*, and *spin/lbfgs* replace the force tolerance *ftol* by a torque tolerance. The minimization procedure stops if the 2-norm (length) of the torque vector on atom (defined as the cross product between the atomic spin and its precession vectors omega) is less than *ftol*, or if any of the other criteria are met. Torque have the same units as the energy.

Note: You can also use the *fix halt* command to specify a general criterion for exiting a minimization, that is a calculation performed on the state of the current system, as defined by an *equal-style variable*.

For the first criterion, the specified energy tolerance *etol* is unitless; it is met when the energy change between successive iterations divided by the energy magnitude is less than or equal to the tolerance. For example, a setting of 1.0e-4 for *etol* means an energy tolerance of one part in 10^4. For the damped dynamics minimizers this check is not performed for a few steps after velocities are reset to 0, otherwise the minimizer would prematurely converge.

For the second criterion, the specified force tolerance *ftol* is in force units, since it is the length of the global force vector for all atoms, e.g. a vector of size 3N for N atoms. Since many of the components will be near zero after minimization, you can think of *ftol* as an upper bound on the final force on any component of any atom. For example, a setting of 1.0e-4 for *ftol* means no x, y, or z component of force on any atom will be larger than 1.0e-4 (in force units) after minimization.

Either or both of the *etol* and *ftol* values can be set to 0.0, in which case some other criterion will terminate the minimization.

During a minimization, the outer iteration count is treated as a timestep. Output is triggered by this timestep, e.g. thermodynamic output or dump and restart files.

Using the *thermo_style custom* command with the *fmax* or *fnorm* keywords can be useful for monitoring the progress of the minimization. Note that these outputs will be calculated only from forces on the atoms, and will not include any extra degrees of freedom, such as from the *fix box/relax* command.

Following minimization, a statistical summary is printed that lists which convergence criterion caused the minimizer to stop, as well as information about the energy, force, final line search, and iteration counts. An example is as follows:

```
Minimization stats:
  Stopping criterion = max iterations
  Energy initial, next-to-last, final =
       -0.626828169302     -2.82642039062     -2.82643549739
  Force two-norm initial, final = 2052.1 91.9642
```

(continues on next page)

(continued from previous page)

```
Force max component initial, final = 346.048 9.78056
Final line search alpha, max atom move = 2.23899e-06 2.18986e-05
Iterations, force evaluations = 2000 12724
```

The 3 energy values are for before and after the minimization and on the next-to-last iteration. This is what the *etol* parameter checks.

The two-norm force values are the length of the global force vector before and after minimization. This is what the *ftol* parameter checks.

The max-component force values are the absolute value of the largest component (x,y,z) in the global force vector, i.e. the infinity-norm of the force vector.

The alpha parameter for the line-search, when multiplied by the max force component (on the last iteration), gives the max distance any atom moved during the last iteration. Alpha will be 0.0 if the line search could not reduce the energy. Even if alpha is non-zero, if the "max atom move" distance is tiny compared to typical atom coordinates, then it is possible the last iteration effectively caused no atom movement and thus the evaluated energy did not change and the minimizer terminated. Said another way, even with non-zero forces, it's possible the effect of those forces is to move atoms a distance less than machine precision, so that the energy cannot be further reduced.

The iterations and force evaluation values are what is checked by the *maxiter* and *maxeval* parameters.

Note: There are several force fields in LAMMPS which have discontinuities or other approximations which may prevent you from performing an energy minimization to high tolerances. For example, you should use a *pair style* that goes to 0.0 at the cutoff distance when performing minimization (even if you later change it when running dynamics). If you do not do this, the total energy of the system will have discontinuities when the relative distance between any pair of atoms changes from cutoff+epsilon to cutoff-epsilon and the minimizer may behave poorly. Some of the many-body potentials use splines and other internal cutoffs that inherently have this problem. The *long-range Coulombic styles* (PPPM, Ewald) are approximate to within the user-specified tolerance, which means their energy and forces may not agree to a higher precision than the Kspace-specified tolerance. In all these cases, the minimizer may give up and stop before finding a minimum to the specified energy or force tolerance.

Note that a cutoff Lennard-Jones potential (and others) can be shifted so that its energy is 0.0 at the cutoff via the *pair_modify* command. See the doc pages for individual *pair styles* for details. Note that Coulombic potentials always have a cutoff, unless versions with a long-range component are used (e.g. *pair_style lj/cut/coul/long*). The CHARMM potentials go to 0.0 at the cutoff (e.g. *pair_style lj/charmm/coul/charmm*), as do the GROMACS potentials (e.g. *pair_style lj/gromacs*).

If a soft potential (*pair_style soft*) is used the Astop value is used for the prefactor (no time dependence).

The *fix box/relax* command can be used to apply an external pressure to the simulation box and allow it to shrink/expand during the minimization.

Only a few other fixes (typically those that add forces) are invoked during minimization. See the doc pages for individual *fix* commands to see which ones are relevant. Current examples of fixes that can be used include:

- *fix addforce*
- *fix addtorque*
- *fix efield*
- *fix enforce2d*
- *fix indent*
- *fix lineforce*

- *fix planeforce*
- *fix setforce*
- *fix spring*
- *fix spring/self*
- *fix viscous*
- *fix wall*
- *fix wall/region*

Note: Some fixes which are invoked during minimization have an associated potential energy. For that energy to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the *fix_modify energy* option for that fix. The doc pages for individual *fix* commands specify if this should be done.

Note: The minimizers in LAMMPS do not allow for bonds (or angles, etc) to be held fixed while atom coordinates are being relaxed, e.g. via *fix shake* or *fix rigid*. See more info in the Restrictions section below.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

15.78.4 Restrictions

Features that are not yet implemented are listed here, in case someone knows how they could be coded:

It is an error to use *fix shake* with minimization because it turns off bonds that should be included in the potential energy of the system. The effect of a fix shake can be approximated during a minimization by using stiff spring constants for the bonds and/or angles that would normally be constrained by the SHAKE algorithm.

Fix rigid is also not supported by minimization. It is not an error to have it defined, but the energy minimization will not keep the defined body(s) rigid during the minimization. Note that if bonds, angles, etc internal to a rigid body have been turned off (e.g. via *neigh_modify exclude*), they will not contribute to the potential energy which is probably not what is desired.

Pair potentials that produce torque on a particle (e.g. *granular potentials* or the *GayBerne potential* for ellipsoidal particles) are not relaxed by a minimization. More specifically, radial relaxations are induced, but no rotations are induced by a minimization, so such a system will not fully relax.

15.78.5 Related commands

min_modify, *min_style*, *run_style*

Default: none

15.79 molecule command

15.79.1 Syntax

```
molecule ID file1 keyword values ... file2 keyword values ... fileN ...
```

- ID = user-assigned name for the molecule template
- file1,file2,... = names of files containing molecule descriptions
- zero or more keyword/value pairs may be appended after each file
- keyword = *offset* or *toff* or *boff* or *aoff* or *doff* or *ioff* or *scale*

```
offset values = Toff Boff Aoff Doff Ioff
  Toff = offset to add to atom types
  Boff = offset to add to bond types
  Aoff = offset to add to angle types
  Doff = offset to add to dihedral types
  Ioff = offset to add to improper types
toff value = Toff
  Toff = offset to add to atom types
boff value = Boff
  Boff = offset to add to bond types
aoff value = Aoff
  Aoff = offset to add to angle types
doff value = Doff
  Doff = offset to add to dihedral types
ioff value = Ioff
  Ioff = offset to add to improper types
scale value = sfactor
  sfactor = scale factor to apply to the size and mass of the molecule
```

15.79.2 Examples

```
molecule 1 mymol.txt
molecule 1 co2.txt h2o.txt
molecule CO2 co2.txt boff 3 aoff 2
molecule 1 mymol.txt offset 6 9 18 23 14
molecule objects file.1 scale 1.5 file.1 scale 2.0 file.2 scale 1.3
```

15.79.3 Description

Define a molecule template that can be used as part of other LAMMPS commands, typically to define a collection of particles as a bonded molecule or a rigid body. Commands that currently use molecule templates include:

- *fix deposit*
- *fix pour*
- *fix rigid/small*
- *fix shake*
- *fix gcmc*
- *create_atoms*
- *atom_style template*

The ID of a molecule template can only contain alphanumeric characters and underscores.

A single template can contain multiple molecules, listed one per file. Some of the commands listed above currently use only the first molecule in the template, and will issue a warning if the template contains multiple molecules. The *atom_style template* command allows multiple-molecule templates to define a system with more than one templated molecule.

Each filename can be followed by optional keywords which are applied only to the molecule in the file as used in this template. This is to make it easy to use the same molecule file in different molecule templates or in different simulations. You can specify the same file multiple times with different optional keywords.

The *offset*, *toff*, *aoff*, *doff*, *ioff* keywords add the specified offset values to the atom types, bond types, angle types, dihedral types, and/or improper types as they are read from the molecule file. E.g. if *toff* = 2, and the file uses atom types 1,2,3, then each created molecule will have atom types 3,4,5. For the *offset* keyword, all five offset values must be specified, but individual values will be ignored if the molecule template does not use that attribute (e.g. no bonds).

The *scale* keyword scales the size of the molecule. This can be useful for modeling polydisperse granular rigid bodies. The scale factor is applied to each of these properties in the molecule file, if they are defined: the individual particle coordinates (Coords section), the individual mass of each particle (Masses section), the individual diameters of each particle (Diameters section), the total mass of the molecule (header keyword = mass), the center-of-mass of the molecule (header keyword = com), and the moments of inertia of the molecule (header keyword = inertia).

Note: The molecule command can be used to define molecules with bonds, angles, dihedrals, impropers, or special bond lists of neighbors within a molecular topology, so that you can later add the molecules to your simulation, via one or more of the commands listed above. Since this topology-related information requires that suitable storage is reserved when LAMMPS creates the simulation box (e.g. when using the *create_box* command or the *read_data* command) suitable space has to be reserved so you do not overflow those pre-allocated data structures when adding molecules later. Both the *create_box* command and the *read_data* command have "extra" options which insure space is allocated for storing topology info for molecules that are added later.

The format of an individual molecule file is similar but (not identical) to the data file read by the *read_data* commands, and is as follows.

A molecule file has a header and a body. The header appears first. The first line of the header is always skipped; it typically contains a description of the file. Then lines are read one at a time. Lines can have a trailing comment starting with '#' that is ignored. If the line is blank (only white-space after comment is deleted), it is skipped. If the line contains a header keyword, the corresponding value(s) is read from the line. If it doesn't contain a header keyword, the line begins the body of the file.

The body of the file contains zero or more sections. The first line of a section has only a keyword. The next line is skipped. The remaining lines of the section contain values. The number of lines depends on the section keyword as

described below. Zero or more blank lines can be used between sections. Sections can appear in any order, with a few exceptions as noted below.

These are the recognized header keywords. Header lines can come in any order. The numeric value(s) are read from the beginning of the line. The keyword should appear at the end of the line. All these settings have default values, as explained below. A line need only appear if the value(s) are different than the default.

- N *atoms* = # of atoms N in molecule, default = 0
- Nb *bonds* = # of bonds Nb in molecule, default = 0
- Na *angles* = # of angles Na in molecule, default = 0
- Nd *dihedrals* = # of dihedrals Nd in molecule, default = 0
- Ni *impropers* = # of impropers Ni in molecule, default = 0
- Mtotal *mass* = total mass of molecule
- Xc Yc Zc *com* = coordinates of center-of-mass of molecule
- Ixx Iyy Izz Ixy Ixz Iyz *inertia* = 6 components of inertia tensor of molecule

For *mass*, *com*, and *inertia*, the default is for LAMMPS to calculate this quantity itself if needed, assuming the molecules consists of a set of point particles or finite-size particles (with a non-zero diameter) that do not overlap. If finite-size particles in the molecule do overlap, LAMMPS will not account for the overlap effects when calculating any of these 3 quantities, so you should pre-compute them yourself and list the values in the file.

The mass and center-of-mass coordinates (Xc,Yc,Zc) are self-explanatory. The 6 moments of inertia (ixx,iyy,izz,ixy,ixz,iyz) should be the values consistent with the current orientation of the rigid body around its center of mass. The values are with respect to the simulation box XYZ axes, not with respect to the principal axes of the rigid body itself. LAMMPS performs the latter calculation internally.

These are the allowed section keywords for the body of the file.

- *Coords, Types, Charges, Diameters, Masses* = atom-property sections
- *Bonds, Angles, Dihedrals, Impropers* = molecular topology sections
- *Special Bond Counts, Special Bonds* = special neighbor info
- *Shake Flags, Shake Atoms, Shake Bond Types* = SHAKE info

If a Bonds section is specified then the Special Bond Counts and Special Bonds sections can also be used, if desired, to explicitly list the 1-2, 1-3, 1-4 neighbors within the molecule topology (see details below). This is optional since if these sections are not included, LAMMPS will auto-generate this information. Note that LAMMPS uses this info to properly exclude or weight bonded pairwise interactions between bonded atoms. See the *special_bonds* command for more details. One reason to list the special bond info explicitly is for the *thermalized Drude oscillator model* which treats the bonds between nuclear cores and Drude electrons in a different manner.

Note: Whether a section is required depends on how the molecule template is used by other LAMMPS commands. For example, to add a molecule via the *fix deposit* command, the Coords and Types sections are required. To add a rigid body via the *fix pour* command, the Bonds (Angles, etc) sections are not required, since the molecule will be treated as a rigid body. Some sections are optional. For example, the *fix pour* command can be used to add "molecules" which are clusters of finite-size granular particles. If the Diameters section is not specified, each particle in the molecule will have a default diameter of 1.0. See the doc pages for LAMMPS commands that use molecule templates for more details.

Each section is listed below in alphabetic order. The format of each section is described including the number of lines it must contain and rules (if any) for whether it can appear in the data file. In each case the ID is ignored; it is simply included for readability, and should be a number from 1 to Nlines for the section, indicating which atom (or bond, etc)

the entry applies to. The lines are assumed to be listed in order from 1 to Nlines, but LAMMPS does not check for this.

Coords section:

- one line per atom
- line syntax: ID x y z
- x,y,z = coordinate of atom

Types section:

- one line per atom
- line syntax: ID type
- type = atom type of atom

Charges section:

- one line per atom
- line syntax: ID q
- q = charge on atom

This section is only allowed for *atom styles* that support charge. If this section is not included, the default charge on each atom in the molecule is 0.0.

Diameters section:

- one line per atom
- line syntax: ID diam
- diam = diameter of atom

This section is only allowed for *atom styles* that support finite-size spherical particles, e.g. atom_style sphere. If not listed, the default diameter of each atom in the molecule is 1.0.

Masses section:

- one line per atom
- line syntax: ID mass
- mass = mass of atom

This section is only allowed for *atom styles* that support per-atom mass, as opposed to per-type mass. See the *mass* command for details. If this section is not included, the default mass for each atom is derived from its volume (see Diameters section) and a default density of 1.0, in *units* of mass/volume.

Bonds section:

- one line per bond

- line syntax: ID type atom1 atom2
- type = bond type (1-Nbondtype)
- atom1,atom2 = IDs of atoms in bond

The IDs for the two atoms in each bond should be values from 1 to Natoms, where Natoms = # of atoms in the molecule.

Angles section:

- one line per angle
- line syntax: ID type atom1 atom2 atom3
- type = angle type (1-Nangletype)
- atom1,atom2,atom3 = IDs of atoms in angle

The IDs for the three atoms in each angle should be values from 1 to Natoms, where Natoms = # of atoms in the molecule. The 3 atoms are ordered linearly within the angle. Thus the central atom (around which the angle is computed) is the atom2 in the list.

Dihedrals section:

- one line per dihedral
- line syntax: ID type atom1 atom2 atom3 atom4
- type = dihedral type (1-Ndihedraltype)
- atom1,atom2,atom3,atom4 = IDs of atoms in dihedral

The IDs for the four atoms in each dihedral should be values from 1 to Natoms, where Natoms = # of atoms in the molecule. The 4 atoms are ordered linearly within the dihedral.

Impropers section:

- one line per improper
- line syntax: ID type atom1 atom2 atom3 atom4
- type = improper type (1-Nimpropertype)
- atom1,atom2,atom3,atom4 = IDs of atoms in improper

The IDs for the four atoms in each improper should be values from 1 to Natoms, where Natoms = # of atoms in the molecule. The ordering of the 4 atoms determines the definition of the improper angle used in the formula for the defined *improper style*. See the doc pages for individual styles for details.

Special Bond Counts section:

- one line per atom
- line syntax: ID N1 N2 N3
- N1 = # of 1-2 bonds
- N2 = # of 1-3 bonds
- N3 = # of 1-4 bonds

N1, N2, N3 are the number of 1-2, 1-3, 1-4 neighbors respectively of this atom within the topology of the molecule. See the *special_bonds* doc page for more discussion of 1-2, 1-3, 1-4 neighbors. If this section appears, the Special Bonds section must also appear.

As explained above, LAMMPS will auto-generate this information if this section is not specified. If specified, this section will override what would be auto-generated.

Special Bonds section:

- one line per atom
- line syntax: ID a b c d . . .
- a,b,c,d,. . . = IDs of atoms in N1+N2+N3 special bonds

A, b, c, d, etc are the IDs of the n1+n2+n3 atoms that are 1-2, 1-3, 1-4 neighbors of this atom. The IDs should be values from 1 to Natoms, where Natoms = # of atoms in the molecule. The first N1 values should be the 1-2 neighbors, the next N2 should be the 1-3 neighbors, the last N3 should be the 1-4 neighbors. No atom ID should appear more than once. See the *special_bonds* doc page for more discussion of 1-2, 1-3, 1-4 neighbors. If this section appears, the Special Bond Counts section must also appear.

As explained above, LAMMPS will auto-generate this information if this section is not specified. If specified, this section will override what would be auto-generated.

Shake Flags section:

- one line per atom
- line syntax: ID flag
- flag = 0,1,2,3,4

This section is only needed when molecules created using the template will be constrained by SHAKE via the "fix shake" command. The other two Shake sections must also appear in the file, following this one.

The meaning of the flag for each atom is as follows. See the *fix shake* doc page for a further description of SHAKE clusters.

- 0 = not part of a SHAKE cluster
- 1 = part of a SHAKE angle cluster (two bonds and the angle they form)
- 2 = part of a 2-atom SHAKE cluster with a single bond
- 3 = part of a 3-atom SHAKE cluster with two bonds
- 4 = part of a 4-atom SHAKE cluster with three bonds

Shake Atoms section:

- one line per atom
- line syntax: ID a b c d
- a,b,c,d = IDs of atoms in cluster

This section is only needed when molecules created using the template will be constrained by SHAKE via the "fix shake" command. The other two Shake sections must also appear in the file.

The a,b,c,d values are atom IDs (from 1 to Natoms) for all the atoms in the SHAKE cluster that this atom belongs to. The number of values that must appear is determined by the shake flag for the atom (see the Shake Flags section above). All atoms in a particular cluster should list their a,b,c,d values identically.

If flag = 0, no a,b,c,d values are listed on the line, just the (ignored) ID.

If flag = 1, a,b,c are listed, where a = ID of central atom in the angle, and b,c the other two atoms in the angle.

If flag = 2, a,b are listed, where a = ID of atom in bond with the lowest ID, and b = ID of atom in bond with the highest ID.

If flag = 3, a,b,c are listed, where a = ID of central atom, and b,c = IDs of other two atoms bonded to the central atom.

If flag = 4, a,b,c,d are listed, where a = ID of central atom, and b,c,d = IDs of other three atoms bonded to the central atom.

See the *fix shake* doc page for a further description of SHAKE clusters.

Shake Bond Types section:

- one line per atom
- line syntax: ID a b c
- a,b,c = bond types (or angle type) of bonds (or angle) in cluster

This section is only needed when molecules created using the template will be constrained by SHAKE via the "fix shake" command. The other two Shake sections must also appear in the file.

The a,b,c values are bond types (from 1 to Nbondtypes) for all bonds in the SHAKE cluster that this atom belongs to. The number of values that must appear is determined by the shake flag for the atom (see the Shake Flags section above). All atoms in a particular cluster should list their a,b,c values identically.

If flag = 0, no a,b,c values are listed on the line, just the (ignored) ID.

If flag = 1, a,b,c are listed, where a = bondtype of the bond between the central atom and the first non-central atom (value b in the Shake Atoms section), b = bondtype of the bond between the central atom and the 2nd non-central atom (value c in the Shake Atoms section), and c = the angle type (1 to Nangletypes) of the angle between the 3 atoms.

If flag = 2, only a is listed, where a = bondtype of the bond between the 2 atoms in the cluster.

If flag = 3, a,b are listed, where a = bondtype of the bond between the central atom and the first non-central atom (value b in the Shake Atoms section), and b = bondtype of the bond between the central atom and the 2nd non-central atom (value c in the Shake Atoms section).

If flag = 4, a,b,c are listed, where a = bondtype of the bond between the central atom and the first non-central atom (value b in the Shake Atoms section), b = bondtype of the bond between the central atom and the 2nd non-central atom (value c in the Shake Atoms section), and c = bondtype of the bond between the central atom and the 3rd non-central atom (value d in the Shake Atoms section).

See the *fix shake* doc page for a further description of SHAKE clusters.

15.79.4 Restrictions

This command must come after the simulation box is define by a *read_data*, *read_restart*, or *create_box* command.

15.79.5 Related commands

fix deposit, *fix pour*, *fix gcmc*

15.79.6 Default

The default keywords values are offset 0 0 0 0 0 and scale = 1.0.

15.80 neb command

15.80.1 Syntax

```
neb etol ftol N1 N2 Nevery file-style arg keyword
```

- etol = stopping tolerance for energy (energy units)
- ftol = stopping tolerance for force (force units)
- N1 = max # of iterations (timesteps) to run initial NEB
- N2 = max # of iterations (timesteps) to run barrier-climbing NEB
- Nevery = print replica energies and reaction coordinates every this many timesteps
- file-style = *final* or *each* or *none*

```
final arg = filename
  filename = file with initial coords for final replica
    coords for intermediate replicas are linearly interpolated
    between first and last replica
each arg = filename
  filename = unique filename for each replica (except first)
    with its initial coords
none arg = no argument all replicas assumed to already have
    their initial coords
```

keyword = *verbose*

15.80.2 Examples

```
neb 0.1 0.0 1000 500 50 final coords.final
neb 0.0 0.001 1000 500 50 each coords.initial.$i
neb 0.0 0.001 1000 500 50 none verbose
```

15.80.3 Description

Perform a nudged elastic band (NEB) calculation using multiple replicas of a system. Two or more replicas must be used; the first and last are the end points of the transition path.

NEB is a method for finding both the atomic configurations and height of the energy barrier associated with a transition state, e.g. for an atom to perform a diffusive hop from one energy basin to another in a coordinated fashion with its neighbors. The implementation in LAMMPS follows the discussion in these 4 papers: *(HenkelmanA)*, *(HenkelmanB)*, *(Nakano)* and *(Maras)*.

Each replica runs on a partition of one or more processors. Processor partitions are defined at run-time using the *-partition command-line switch*. Note that if you have MPI installed, you can run a multi-replica simulation with more replicas (partitions) than you have physical processors, e.g you can run a 10-replica simulation on just one or two processors. You will simply not get the performance speed-up you would see with one or more physical processors per replica. See the *Howto replica* doc page for further discussion.

Note: As explained below, a NEB calculation performs a damped dynamics minimization across all the replicas. The minimizer uses whatever timestep you have defined in your input script, via the *timestep* command. Often NEB will converge more quickly if you use a timestep about 10x larger than you would normally use for dynamics simulations.

When a NEB calculation is performed, it is assumed that each replica is running the same system, though LAMMPS does not check for this. I.e. the simulation domain, the number of atoms, the interaction potentials, and the starting configuration when the neb command is issued should be the same for every replica.

In a NEB calculation each replica is connected to other replicas by inter-replica nudging forces. These forces are imposed by the *fix neb* command, which must be used in conjunction with the neb command. The group used to define the fix neb command defines the NEB atoms which are the only ones that inter-replica springs are applied to. If the group does not include all atoms, then non-NEB atoms have no inter-replica springs and the forces they feel and their motion is computed in the usual way due only to other atoms within their replica. Conceptually, the non-NEB atoms provide a background force field for the NEB atoms. They can be allowed to move during the NEB minimization procedure (which will typically induce different coordinates for non-NEB atoms in different replicas), or held fixed using other LAMMPS commands such as *fix setforce*. Note that the *partition* command can be used to invoke a command on a subset of the replicas, e.g. if you wish to hold NEB or non-NEB atoms fixed in only the end-point replicas.

The initial atomic configuration for each of the replicas can be specified in different manners via the *file-style* setting, as discussed below. Only atoms whose initial coordinates should differ from the current configuration need be specified.

Conceptually, the initial and final configurations for the first replica should be states on either side of an energy barrier.

As explained below, the initial configurations of intermediate replicas can be atomic coordinates interpolated in a linear fashion between the first and last replicas. This is often adequate for simple transitions. For more complex transitions, it may lead to slow convergence or even bad results if the minimum energy path (MEP, see below) of states over the barrier cannot be correctly converged to from such an initial path. In this case, you will want to generate initial states for the intermediate replicas that are geometrically closer to the MEP and read them in.

For a *file-style* setting of *final*, a filename is specified which contains atomic coordinates for zero or more atoms, in the format described below. For each atom that appears in the file, the new coordinates are assigned to that atom in the final replica. Each intermediate replica also assigns a new position to that atom in an interpolated manner. This is done by using the current position of the atom as the starting point and the read-in position as the final point. The distance between them is calculated, and the new position is assigned to be a fraction of the distance. E.g. if there are 10 replicas, the 2nd replica will assign a position that is 10% of the distance along a line between the starting and final point, and the 9th replica will assign a position that is 90% of the distance along the line. Note that for this procedure to produce consistent coordinates across all the replicas, the current coordinates need to be the same in all replicas. LAMMPS does not check for this, but invalid initial configurations will likely result if it is not the case.

Note: The "distance" between the starting and final point is calculated in a minimum-image sense for a periodic simulation box. This means that if the two positions are on opposite sides of a box (periodic in that dimension), the distance between them will be small, because the periodic image of one of the atoms is close to the other. Similarly, even if the assigned position resulting from the interpolation is outside the periodic box, the atom will be wrapped back into the box when the NEB calculation begins.

For a *file-style* setting of *each*, a filename is specified which is assumed to be unique to each replica. This can be done by using a variable in the filename, e.g.

```
variable i equal part
neb 0.0 0.001 1000 500 50 each coords.initial.$i
```

which in this case will substitute the partition ID (0 to N-1) for the variable I, which is also effectively the replica ID. See the *variable* command for other options, such as using world-, universe-, or uloop-style variables.

Each replica (except the first replica) will read its file, formatted as described below, and for any atom that appears in the file, assign the specified coordinates to its atom. The various files do not need to contain the same set of atoms.

For a *file-style* setting of *none*, no filename is specified. Each replica is assumed to already be in its initial configuration at the time the neb command is issued. This allows each replica to define its own configuration by reading a replica-specific data or restart or dump file, via the *read_data*, *read_restart*, or *read_dump* commands. The replica-specific names of these files can be specified as in the discussion above for the *each* file-style. Also see the section below for how a NEB calculation can produce restart files, so that a long calculation can be restarted if needed.

Note: None of the *file-style* settings change the initial configuration of any atom in the first replica. The first replica must thus be in the correct initial configuration at the time the neb command is issued.

A NEB calculation proceeds in two stages, each of which is a minimization procedure, performed via damped dynamics. To enable this, you must first define a damped dynamics *min_style*, such as *quickmin* or *fire*. The *cg*, *sd*, and *hftn* styles cannot be used, since they perform iterative line searches in their inner loop, which cannot be easily synchronized across multiple replicas.

The minimizer tolerances for energy and force are set by *etol* and *ftol*, the same as for the *minimize* command.

A non-zero *etol* means that the NEB calculation will terminate if the energy criterion is met by every replica. The energies being compared to *etol* do not include any contribution from the inter-replica nudging forces, since these are non-conservative. A non-zero *ftol* means that the NEB calculation will terminate if the force criterion is met by every replica. The forces being compared to *ftol* include the inter-replica nudging forces.

The maximum number of iterations in each stage is set by *N1* and *N2*. These are effectively timestep counts since each iteration of damped dynamics is like a single timestep in a dynamics *run*. During both stages, the potential energy of each replica and its normalized distance along the reaction path (reaction coordinate RD) will be printed to the screen and log file every *Nevery* timesteps. The RD is 0 and 1 for the first and last replica. For intermediate replicas, it is the cumulative distance (normalized by the total cumulative distance) between adjacent replicas, where "distance" is defined as the length of the 3N-vector of differences in atomic coordinates, where N is the number of NEB atoms involved in the transition. These outputs allow you to monitor NEB's progress in finding a good energy barrier. *N1* and *N2* must both be multiples of *Nevery*.

In the first stage of NEB, the set of replicas should converge toward a minimum energy path (MEP) of conformational states that transition over a barrier. The MEP for a transition is defined as a sequence of 3N-dimensional states, each of which has a potential energy gradient parallel to the MEP itself. The configuration of highest energy along a MEP corresponds to a saddle point. The replica states will also be roughly equally spaced along the MEP due to the inter-replica nudging force added by the *fix neb* command.

In the second stage of NEB, the replica with the highest energy is selected and the inter-replica forces on it are converted to a force that drives its atom coordinates to the top or saddle point of the barrier, via the barrier-climbing calculation described in *(HenkelmanB)*. As before, the other replicas rearrange themselves along the MEP so as to be roughly equally spaced.

When both stages are complete, if the NEB calculation was successful, the configurations of the replicas should be along (close to) the MEP and the replica with the highest energy should be an atomic configuration at (close to) the saddle point of the transition. The potential energies for the set of replicas represents the energy profile of the transition along the MEP.

A few other settings in your input script are required or advised to perform a NEB calculation. See the NOTE about the choice of timestep at the beginning of this doc page.

An atom map must be defined which it is not by default for *atom_style atomic* problems. The *atom_modify map* command can be used to do this.

The minimizers in LAMMPS operate on all atoms in your system, even non-NEB atoms, as defined above. To prevent non-NEB atoms from moving during the minimization, you should use the *fix setforce* command to set the force on each of those atoms to 0.0. This is not required, and may not even be desired in some cases, but if those atoms move too far (e.g. because the initial state of your system was not well-minimized), it can cause problems for the NEB procedure.

The damped dynamics *minimizers*, such as *quickmin* and *fire*), adjust the position and velocity of the atoms via an Euler integration step. Thus you must define an appropriate *timestep* to use with NEB. As mentioned above, NEB will often converge more quickly if you use a timestep about 10x larger than you would normally use for dynamics simulations.

Each file read by the neb command containing atomic coordinates used to initialize one or more replicas must be formatted as follows.

The file can be ASCII text or a gzipped text file (detected by a .gz suffix). The file can contain initial blank lines or comment lines starting with "#" which are ignored. The first non-blank, non-comment line should list N = the number of lines to follow. The N successive lines contain the following information:

```
ID1 x1 y1 z1
ID2 x2 y2 z2
...
IDN xN yN zN
```

The fields are the atom ID, followed by the x,y,z coordinates. The lines can be listed in any order. Additional trailing information on the line is OK, such as a comment.

Note that for a typical NEB calculation you do not need to specify initial coordinates for very many atoms to produce differing starting and final replicas whose intermediate replicas will converge to the energy barrier. Typically only new coordinates for atoms geometrically near the barrier need be specified.

Also note there is no requirement that the atoms in the file correspond to the NEB atoms in the group defined by the *fix neb* command. Not every NEB atom need be in the file, and non-NEB atoms can be listed in the file.

Four kinds of output can be generated during a NEB calculation: energy barrier statistics, thermodynamic output by each replica, dump files, and restart files.

When running with multiple partitions (each of which is a replica in this case), the print-out to the screen and master log.lammps file contains a line of output, printed once every *Nevery* timesteps. It contains the timestep, the maximum force per replica, the maximum force per atom (in any replica), potential gradients in the initial, final, and climbing

replicas, the forward and backward energy barriers, the total reaction coordinate (RDT), and the normalized reaction coordinate and potential energy of each replica.

The "maximum force per replica" is the two-norm of the 3N-length force vector for the atoms in each replica, maximized across replicas, which is what the *ftol* setting is checking against. In this case, N is all the atoms in each replica. The "maximum force per atom" is the maximum force component of any atom in any replica. The potential gradients are the two-norm of the 3N-length force vector solely due to the interaction potential i.e. without adding in inter-replica forces.

The "reaction coordinate" (RD) for each replica is the two-norm of the 3N-length vector of distances between its atoms and the preceding replica's atoms, added to the RD of the preceding replica. The RD of the first replica RD1 = 0.0; the RD of the final replica RDN = RDT, the total reaction coordinate. The normalized RDs are divided by RDT, so that they form a monotonically increasing sequence from zero to one. When computing RD, N only includes the atoms being operated on by the fix neb command.

The forward (reverse) energy barrier is the potential energy of the highest replica minus the energy of the first (last) replica.

Supplementary information for all replicas can be printed out to the screen and master log.lammps file by adding the verbose keyword. This information include the following. The "path angle" (pathangle) for the replica i which is the angle between the 3N-length vectors (Ri-1 - Ri) and (Ri+1 - Ri) (where Ri is the atomic coordinates of replica i). A "path angle" of 180 indicates that replicas i-1, i and i+1 are aligned. "angletangrad" is the angle between the 3N-length tangent vector and the 3N-length force vector at image i. The tangent vector is calculated as in *(HenkelmanA)* for all intermediate replicas and at R2 - R1 and RM - RM-1 for the first and last replica, respectively. "anglegrad" is the angle between the 3N-length energy gradient vector of replica i and that of replica i+1. It is not defined for the final replica and reads nan. gradV is the norm of the energy gradient of image i. ReplicaForce is the two-norm of the 3N-length force vector (including nudging forces) for replica i. MaxAtomForce is the maximum force component of any atom in replica i.

When a NEB calculation does not converge properly, the supplementary information can help understanding what is going wrong. For instance when the path angle becomes acute, the definition of tangent used in the NEB calculation is questionable and the NEB cannot may diverge *(Maras)*.

When running on multiple partitions, LAMMPS produces additional log files for each partition, e.g. log.lammps.0, log.lammps.1, etc. For a NEB calculation, these contain the thermodynamic output for each replica.

If *dump* commands in the input script define a filename that includes a *universe* or *uloop* style *variable*, then one dump file (per dump command) will be created for each replica. At the end of the NEB calculation, the final snapshot in each file will contain the sequence of snapshots that transition the system over the energy barrier. Earlier snapshots will show the convergence of the replicas to the MEP.

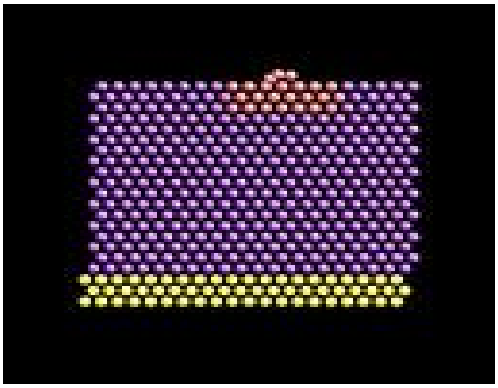
Likewise, *restart* filenames can be specified with a *universe* or *uloop* style *variable*, to generate restart files for each replica. These may be useful if the NEB calculation fails to converge properly to the MEP, and you wish to restart the calculation from an intermediate point with altered parameters.

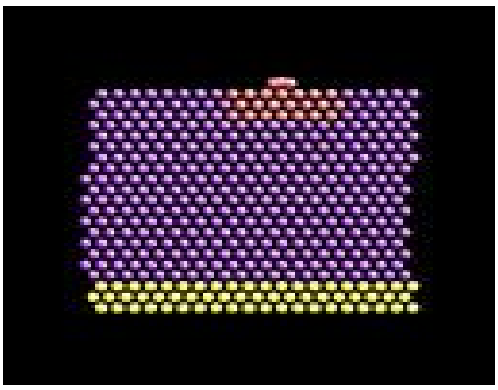
There are 2 Python scripts provided in the tools/python directory, neb_combine.py and neb_final.py, which are useful in analyzing output from a NEB calculation. Assume a NEB simulation with M replicas, and the NEB atoms labeled with a specific atom type.

The neb_combine.py script extracts atom coords for the NEB atoms from all M dump files and creates a single dump file where each snapshot contains the NEB atoms from all the replicas and one copy of non-NEB atoms from the first replica (presumed to be identical in other replicas). This can be visualized/animated to see how the NEB atoms relax as the NEB calculation proceeds.

The neb_final.py script extracts the final snapshot from each of the M dump files to create a single dump file with M snapshots. This can be visualized to watch the system make its transition over the energy barrier.

To illustrate, here are images from the final snapshot produced by the neb_combine.py script run on the dump files produced by the two example input scripts in examples/neb. Click on them to see a larger image.





15.80.4 Restrictions

This command can only be used if LAMMPS was built with the REPLICA package. See the *Build package* doc page for more info.

15.80.5 Related commands

prd, *temper*, *fix langevin*, *fix viscous*

15.80.6 Default

none

(HenkelmanA) Henkelman and Jonsson, J Chem Phys, 113, 9978-9985 (2000).

(HenkelmanB) Henkelman, Uberuaga, Jonsson, J Chem Phys, 113, 9901-9904 (2000).

(Nakano) Nakano, Comp Phys Comm, 178, 280-289 (2008).

(Maras) Maras, Trushin, Stukowski, Ala-Nissila, Jonsson, Comp Phys Comm, 205, 13-21 (2016)

15.81 neb/spin command

15.81.1 Syntax

```
neb/spin etol ttol N1 N2 Nevery file-style arg keyword
```

- etol = stopping tolerance for energy (energy units)
- ttol = stopping tolerance for torque (units)
- N1 = max # of iterations (timesteps) to run initial NEB
- N2 = max # of iterations (timesteps) to run barrier-climbing NEB
- Nevery = print replica energies and reaction coordinates every this many timesteps
- file-style = *final* or *each* or *none*

```
final arg = filename
  filename = file with initial coords for final replica
    coords for intermediate replicas are linearly interpolated
    between first and last replica
each arg = filename
  filename = unique filename for each replica (except first)
    with its initial coords
none arg = no argument all replicas assumed to already have
    their initial coords
```

- keyword = *verbose*

```
verbose = print supplemental information
```

15.81.2 Examples

```
neb/spin 0.1 0.0 1000 500 50 final coords.final
neb/spin 0.0 0.001 1000 500 50 each coords.initial.$i
neb/spin 0.0 0.001 1000 500 50 none verbose
```

15.81.3 Description

Perform a geodesic nudged elastic band (GNEB) calculation using multiple replicas of a system. Two or more replicas must be used; the first and last are the end points of the transition path.

GNEB is a method for finding both the spin configurations and height of the energy barrier associated with a transition state, e.g. spins to perform a collective rotation from one energy basin to another. The implementation in LAMMPS follows the discussion in the following paper: *(BessarabA)*.

Each replica runs on a partition of one or more processors. Processor partitions are defined at run-time using the *-partition command-line switch*. Note that if you have MPI installed, you can run a multi-replica simulation with more replicas (partitions) than you have physical processors, e.g you can run a 10-replica simulation on just one or two processors. You will simply not get the performance speed-up you would see with one or more physical processors per replica. See the *Howto replica* doc page for further discussion.

Note: As explained below, a GNEB calculation performs a minimization across all the replicas. One of the *spin* style minimizers has to be defined in your input script.

When a GNEB calculation is performed, it is assumed that each replica is running the same system, though LAMMPS does not check for this. I.e. the simulation domain, the number of magnetic atoms, the interaction potentials, and the starting configuration when the neb command is issued should be the same for every replica.

In a GNEB calculation each replica is connected to other replicas by inter-replica nudging forces. These forces are imposed by the *fix neb/spin* command, which must be used in conjunction with the neb command. The group used to define the fix neb/spin command defines the GNEB magnetic atoms which are the only ones that inter-replica springs are applied to. If the group does not include all magnetic atoms, then non-GNEB magnetic atoms have no inter-replica springs and the torques they feel and their precession motion is computed in the usual way due only to other magnetic atoms within their replica. Conceptually, the non-GNEB atoms provide a background force field for the GNEB atoms. Their magnetic spins can be allowed to evolve during the GNEB minimization procedure.

The initial spin configuration for each of the replicas can be specified in different manners via the *file-style* setting, as discussed below. Only atomic spins whose initial coordinates should differ from the current configuration need to be specified.

Conceptually, the initial and final configurations for the first replica should be states on either side of an energy barrier.

As explained below, the initial configurations of intermediate replicas can be spin coordinates interpolated in a linear fashion between the first and last replicas. This is often adequate for simple transitions. For more complex transitions, it may lead to slow convergence or even bad results if the minimum energy path (MEP, see below) of states over the barrier cannot be correctly converged to from such an initial path. In this case, you will want to generate initial states for the intermediate replicas that are geometrically closer to the MEP and read them in.

For a *file-style* setting of *final*, a filename is specified which contains atomic and spin coordinates for zero or more atoms, in the format described below. For each atom that appears in the file, the new coordinates are assigned to that atom in the final replica. Each intermediate replica also assigns a new spin to that atom in an interpolated manner. This is done by using the current direction of the spin at the starting point and the read-in direction as the final point. The "angular distance" between them is calculated, and the new direction is assigned to be a fraction of the angular distance.

Note: The "angular distance" between the starting and final point is evaluated in the geodesic sense, as described in *(BessarabA)*.

Note: The angular interpolation between the starting and final point is achieved using Rodrigues formula:

$$\vec{m}_i^\nu = \vec{m}_i^I \cos(\omega_i^\nu) + (\vec{k}_i \times \vec{m}_i^I)\sin(\omega_i^\nu) + (1.0 - \cos(\omega_i^\nu))\vec{k}_i(\vec{k}_i \cdot \vec{m}_i^I)$$

where $\vec{m}_i^I$ is the initial spin configuration for spin i, ω_i^ν is a rotation angle defined as:

$$\omega_i^\nu = (\nu - 1)\Delta\omega_i \text{ and } \Delta\omega_i = \frac{\omega_i}{Q-1}$$

with ν the image number, Q the total number of images, and ω_i the total rotation between the initial and final spins. $\vec{k}_i$ defines a rotation axis such as:

$$\vec{k}_i = \frac{\vec{m}_i^I \times \vec{m}_i^F}{\left|\vec{m}_i^I \times \vec{m}_i^F\right|}$$

if the initial and final spins are not aligned. If the initial and final spins are aligned, then their cross product is null, and the expression above does not apply. If they point toward the same direction, the intermediate images conserve the same orientation. If the initial and final spins are aligned, but point toward opposite directions, an arbitrary rotation vector belonging to the plane perpendicular to initial and final spins is chosen. In this case, a warning message is displayed.

For a *file-style* setting of *each*, a filename is specified which is assumed to be unique to each replica. See the *neb* documentation page for more information about this option.

For a *file-style* setting of *none*, no filename is specified. Each replica is assumed to already be in its initial configuration at the time the neb command is issued. This allows each replica to define its own configuration by reading a replica-specific data or restart or dump file, via the *read_data*, *read_restart*, or *read_dump* commands. The replica-specific names of these files can be specified as in the discussion above for the *each* file-style. Also see the section below for how a NEB calculation can produce restart files, so that a long calculation can be restarted if needed.

Note: None of the *file-style* settings change the initial configuration of any atom in the first replica. The first replica must thus be in the correct initial configuration at the time the neb command is issued.

A NEB calculation proceeds in two stages, each of which is a minimization procedure. To enable this, you must first define a *min_style*, using either the *spin*, *spin/cg*, or *spin/lbfgs* style (see *min_spin* for more information). The other styles cannot be used, since they relax the lattice degrees of freedom instead of the spins.

The minimizer tolerances for energy and force are set by *etol* and *ttol*, the same as for the *minimize* command.

A non-zero *etol* means that the GNEB calculation will terminate if the energy criterion is met by every replica. The energies being compared to *etol* do not include any contribution from the inter-replica nudging forces, since these are non-conservative. A non-zero *ttol* means that the GNEB calculation will terminate if the torque criterion is met by every replica. The torques being compared to *ttol* include the inter-replica nudging forces.

The maximum number of iterations in each stage is set by *N1* and *N2*. These are effectively timestep counts since each iteration of damped dynamics is like a single timestep in a dynamics *run*. During both stages, the potential energy of each replica and its normalized distance along the reaction path (reaction coordinate RD) will be printed to the screen and log file every *Nevery* timesteps. The RD is 0 and 1 for the first and last replica. For intermediate replicas, it is the cumulative angular distance (normalized by the total cumulative angular distance) between adjacent replicas, where "distance" is defined as the length of the 3N-vector of the geodesic distances in spin coordinates, with N the number of GNEB spins involved (see equation (13) in *(BessarabA)*). These outputs allow you to monitor NEB's progress in finding a good energy barrier. *N1* and *N2* must both be multiples of *Nevery*.

In the first stage of GNEB, the set of replicas should converge toward a minimum energy path (MEP) of conformational states that transition over a barrier. The MEP for a transition is defined as a sequence of 3N-dimensional spin states, each of which has a potential energy gradient parallel to the MEP itself. The configuration of highest energy along a MEP corresponds to a saddle point. The replica states will also be roughly equally spaced along the MEP due to the inter-replica nudging force added by the *fix neb* command.

In the second stage of GNEB, the replica with the highest energy is selected and the inter-replica forces on it are converted to a force that drives its spin coordinates to the top or saddle point of the barrier, via the barrier-climbing calculation described in *(BessarabA)*. As before, the other replicas rearrange themselves along the MEP so as to be roughly equally spaced.

When both stages are complete, if the GNEB calculation was successful, the configurations of the replicas should be along (close to) the MEP and the replica with the highest energy should be a spin configuration at (close to) the saddle point of the transition. The potential energies for the set of replicas represents the energy profile of the transition along the MEP.

An atom map must be defined which it is not by default for *atom_style atomic* problems. The *atom_modify map* command can be used to do this.

An initial value can be defined for the timestep. Although, the *spin* minimization algorithm is an adaptive timestep methodology, so that this timestep is likely to evolve during the calculation.

The minimizers in LAMMPS operate on all spins in your system, even non-GNEB atoms, as defined above.

Each file read by the neb/spin command containing spin coordinates used to initialize one or more replicas must be formatted as follows.

The file can be ASCII text or a gzipped text file (detected by a .gz suffix). The file can contain initial blank lines or comment lines starting with "#" which are ignored. The first non-blank, non-comment line should list N = the number of lines to follow. The N successive lines contain the following information:

```
ID1 g1 x1 y1 z1 sx1 sy1 sz1
ID2 g2 x2 y2 z2 sx2 sy2 sz2
...
IDN gN yN zN sxN syN szN
```

The fields are the atom ID, the norm of the associated magnetic spin, followed by the *x,y,z* coordinates and the *sx,sy,sz* spin coordinates. The lines can be listed in any order. Additional trailing information on the line is OK, such as a comment.

Note that for a typical GNEB calculation you do not need to specify initial spin coordinates for very many atoms to produce differing starting and final replicas whose intermediate replicas will converge to the energy barrier. Typically only new spin coordinates for atoms geometrically near the barrier need be specified.

Also note there is no requirement that the atoms in the file correspond to the GNEB atoms in the group defined by the *fix neb* command. Not every GNEB atom need be in the file, and non-GNEB atoms can be listed in the file.

Four kinds of output can be generated during a GNEB calculation: energy barrier statistics, thermodynamic output by each replica, dump files, and restart files.

When running with multiple partitions (each of which is a replica in this case), the print-out to the screen and master log.lammps file contains a line of output, printed once every *Nevery* timesteps. It contains the timestep, the maximum torque per replica, the maximum torque per atom (in any replica), potential gradients in the initial, final, and climbing replicas, the forward and backward energy barriers, the total reaction coordinate (RDT), and the normalized reaction coordinate and potential energy of each replica.

The "maximum torque per replica" is the two-norm of the 3N-length vector given by the cross product of a spin by its precession vector omega, in each replica, maximized across replicas, which is what the *ttol* setting is checking against. In this case, N is all the atoms in each replica. The "maximum torque per atom" is the maximum torque component of any atom in any replica. The potential gradients are the two-norm of the 3N-length magnetic precession vector solely due to the interaction potential i.e. without adding in inter-replica forces, and projected along the path tangent (as detailed in Appendix D of *(BessarabA)*).

The "reaction coordinate" (RD) for each replica is the two-norm of the 3N-length vector of geodesic distances between its spins and the preceding replica's spins (see equation (13) of *(BessarabA)*), added to the RD of the preceding replica. The RD of the first replica RD1 = 0.0; the RD of the final replica RDN = RDT, the total reaction coordinate. The normalized RDs are divided by RDT, so that they form a monotonically increasing sequence from zero to one. When computing RD, N only includes the spins being operated on by the fix neb/spin command.

The forward (reverse) energy barrier is the potential energy of the highest replica minus the energy of the first (last) replica.

Supplementary information for all replicas can be printed out to the screen and master log.lammps file by adding the *verbose* keyword. This information include the following. The "GradVidottan" are the projections of the potential

gradient for the replica i on its tangent vector (as detailed in Appendix D of *(BessarabA)*). The "DNi" are the non normalized geodesic distances (see equation (13) of *(BessarabA)*), between a replica i and the next replica i+1. For the last replica, this distance is not defined and a "NAN" value is the corresponding output.

When a NEB calculation does not converge properly, the supplementary information can help understanding what is going wrong.

When running on multiple partitions, LAMMPS produces additional log files for each partition, e.g. log.lammps.0, log.lammps.1, etc. For a GNEB calculation, these contain the thermodynamic output for each replica.

If *dump* commands in the input script define a filename that includes a *universe* or *uloop* style *variable*, then one dump file (per dump command) will be created for each replica. At the end of the GNEB calculation, the final snapshot in each file will contain the sequence of snapshots that transition the system over the energy barrier. Earlier snapshots will show the convergence of the replicas to the MEP.

Likewise, *restart* filenames can be specified with a *universe* or *uloop* style *variable*, to generate restart files for each replica. These may be useful if the GNEB calculation fails to converge properly to the MEP, and you wish to restart the calculation from an intermediate point with altered parameters.

A c file script in provided in the tool/spin/interpolate_gneb directory, that interpolates the MEP given the information provided by the *verbose* output option (as detailed in Appendix D of *(BessarabA)*).

15.81.4 Restrictions

This command can only be used if LAMMPS was built with the SPIN package. See the *Build package* doc page for more info.

For magnetic GNEB calculations, only the *spin_none* value for the *line* keyword can be used when minimization styles *spin/cg* and *spin/lbfgs* are employed.

15.81.5 Related commands

min/spin, *fix neb/spin*

15.81.6 Default

none

(BessarabA) Bessarab, Uzdin, Jonsson, Comp Phys Comm, 196, 335-347 (2015).

15.82 neigh_modify command

15.82.1 Syntax

```
neigh_modify keyword values ...
```

- one or more keyword/value pairs may be listed

```
keyword = delay or every or check or once or cluster or include or␣
↪exclude or page or one or binsize
  delay value = N
    N = delay building until this many steps since last build
  every value = M
    M = build neighbor list every this many steps
  check value = yes or no
    yes = only build if some atom has moved half the skin distance or more
    no = always build on 1st step that every and delay are satisfied
  once
    yes = only build neighbor list once at start of run and never rebuild
    no = rebuild neighbor list according to other settings
  cluster
    yes = check bond,angle,etc neighbor list for nearby clusters
    no = do not check bond,angle,etc neighbor list for nearby clusters
  include value = group-ID
    group-ID = only build pair neighbor lists for atoms in this group
  exclude values:
    type M N
      M,N = exclude if one atom in pair is type M, other is type N
    group group1-ID group2-ID
      group1-ID,group2-ID = exclude if one atom is in 1st group, other in␣
↪2nd
    molecule/intra group-ID
      group-ID = exclude if both atoms are in the same molecule and in␣
↪group
    molecule/inter group-ID
      group-ID = exclude if both atoms are in different molecules and in␣
↪group
    none
      delete all exclude settings
  page value = N
    N = number of pairs stored in a single neighbor page
  one value = N
    N = max number of neighbors of one atom
  binsize value = size
    size = bin size for neighbor list construction (distance units)
```

15.82.2 Examples

```
neigh_modify every 2 delay 10 check yes page 100000
neigh_modify exclude type 2 3
neigh_modify exclude group frozen frozen check no
neigh_modify exclude group residue1 chain3
neigh_modify exclude molecule/intra rigid
```

15.82.3 Description

This command sets parameters that affect the building and use of pairwise neighbor lists. Depending on what pair interactions and other commands are defined, a simulation may require one or more neighbor lists.

The *every*, *delay*, *check*, and *once* options affect how often lists are built as a simulation runs. The *delay* setting means never build new lists until at least N steps after the previous build. The *every* setting means build lists every M steps (after the delay has passed). If the *check* setting is *no*, the lists are built on the first step that satisfies the *delay* and *every* settings. If the *check* setting is *yes*, then the *every* and *delay* settings determine when a build may possibly be performed, but an actual build only occurs if some atom has moved more than half the skin distance (specified in the *neighbor* command) since the last build.

If the *once* setting is yes, then the neighbor list is only built once at the beginning of each run, and never rebuilt, except on steps when a restart file is written, or steps when a fix forces a rebuild to occur (e.g. fixes that create or delete atoms, such as *fix deposit* or *fix evaporate*). This setting should only be made if you are certain atoms will not move far enough that the neighbor list should be rebuilt, e.g. running a simulation of a cold crystal. Note that it is not that expensive to check if neighbor lists should be rebuilt.

When the rRESPA integrator is used (see the *run_style* command), the *every* and *delay* parameters refer to the longest (outermost) timestep.

The *cluster* option does a sanity test every time neighbor lists are built for bond, angle, dihedral, and improper interactions, to check that each set of 2, 3, or 4 atoms is a cluster of nearby atoms. It does this by computing the distance between pairs of atoms in the interaction and insuring they are not further apart than half the periodic box length. If they are, an error is generated, since the interaction would be computed between far-away atoms instead of their nearby periodic images. The only way this should happen is if the pairwise cutoff is so short that atoms that are part of the same interaction are not communicated as ghost atoms. This is an unusual model (e.g. no pair interactions at all) and the problem can be fixed by use of the *comm_modify cutoff* command. Note that to save time, the default *cluster* setting is *no*, so that this check is not performed.

The *include* option limits the building of pairwise neighbor lists to atoms in the specified group. This can be useful for models where a large portion of the simulation is particles that do not interact with other particles or with each other via pairwise interactions. The group specified with this option must also be specified via the *atom_modify first* command. Note that specifying "all" as the group-ID effectively turns off the *include* option.

The *exclude* option turns off pairwise interactions between certain pairs of atoms, by not including them in the neighbor list. These are sample scenarios where this is useful:

- In crack simulations, pairwise interactions can be shut off between 2 slabs of atoms to effectively create a crack.
- When a large collection of atoms is treated as frozen, interactions between those atoms can be turned off to save needless computation. E.g. Using the *fix setforce* command to freeze a wall or portion of a bio-molecule.
- When one or more rigid bodies are specified, interactions within each body can be turned off to save needless computation. See the *fix rigid* command for more details.

The *exclude type* option turns off the pairwise interaction if one atom is of type M and the other of type N. M can equal N. The *exclude group* option turns off the interaction if one atom is in the first group and the other is the second. Group1-ID can equal group2-ID. The *exclude molecule/intra* option turns off the interaction if both atoms are in the specified group and in the same molecule, as determined by their molecule ID. The *exclude molecule/inter* turns off the interaction between pairs of atoms that have different molecule IDs and are both in the specified group.

Each of the exclude options can be specified multiple times. The *exclude type* option is the most efficient option to use; it requires only a single check, no matter how many times it has been specified. The other exclude options are more expensive if specified multiple times; they require one check for each time they have been specified.

Note that the exclude options only affect pairwise interactions; see the *delete_bonds* command for information on turning off bond interactions.

Note: Excluding pairwise interactions will not work correctly when also using a long-range solver via the *kspace_style* command. LAMMPS will give a warning to this effect. This is because the short-range pairwise interaction needs to subtract off a term from the total energy for pairs whose short-range interaction is excluded, to compensate for how the long-range solver treats the interaction. This is done correctly for pairwise interactions that are excluded (or weighted) via the *special_bonds* command. But it is not done for interactions that are excluded via these neigh_modify exclude options.

The *page* and *one* options affect how memory is allocated for the neighbor lists. For most simulations the default settings for these options are fine, but if a very large problem is being run or a very long cutoff is being used, these parameters can be tuned. The indices of neighboring atoms are stored in "pages", which are allocated one after another as they fill up. The size of each page is set by the *page* value. A new page is allocated when the next atom's neighbors could potentially overflow the list. This threshold is set by the *one* value which tells LAMMPS the maximum number of neighbor's one atom can have.

Note: LAMMPS can crash without an error message if the number of neighbors for a single particle is larger than the *page* setting, which means it is much, much larger than the *one* setting. This is because LAMMPS doesn't error check these limits for every pairwise interaction (too costly), but only after all the particle's neighbors have been found. This problem usually means something is very wrong with the way you have setup your problem (particle spacing, cutoff length, neighbor skin distance, etc). If you really expect that many neighbors per particle, then boost the *one* and *page* settings accordingly.

The *binsize* option allows you to specify what size of bins will be used in neighbor list construction to sort and find neighboring atoms. By default, for *neighbor style bin*, LAMMPS uses bins that are 1/2 the size of the maximum pair cutoff. For *neighbor style multi*, the bins are 1/2 the size of the minimum pair cutoff. Typically these are good values for minimizing the time for neighbor list construction. This setting overrides the default. If you make it too big, there is little overhead due to looping over bins, but more atoms are checked. If you make it too small, the optimal number of atoms is checked, but bin overhead goes up. If you set the binsize to 0.0, LAMMPS will use the default binsize of 1/2 the cutoff.

15.82.4 Restrictions

If the "delay" setting is non-zero, then it must be a multiple of the "every" setting.

The molecule/intra and molecule/inter exclude options can only be used with atom styles that define molecule IDs.

The value of the *page* setting must be at least 10x larger than the *one* setting. This insures neighbor pages are not mostly empty space.

15.82.5 Related commands

neighbor, *delete_bonds*

15.82.6 Default

The option defaults are delay = 10, every = 1, check = yes, once = no, cluster = no, include = all (same as no include option defined), exclude = none, page = 100000, one = 2000, and binsize = 0.0.

15.83 neighbor command

15.83.1 Syntax

```
neighbor skin style
```

- skin = extra distance beyond force cutoff (distance units)
- style = *bin* or *nsq* or *multi*

15.83.2 Examples

```
neighbor 0.3 bin
neighbor 2.0 nsq
```

15.83.3 Description

This command sets parameters that affect the building of pairwise neighbor lists. All atom pairs within a neighbor cutoff distance equal to the their force cutoff plus the *skin* distance are stored in the list. Typically, the larger the skin distance, the less often neighbor lists need to be built, but more pairs must be checked for possible force interactions every timestep. The default value for *skin* depends on the choice of units for the simulation; see the default values below.

The *skin* distance is also used to determine how often atoms migrate to new processors if the *check* option of the *neigh_modify* command is set to *yes*. Atoms are migrated (communicated) to new processors on the same timestep that neighbor lists are re-built.

The *style* value selects what algorithm is used to build the list. The *bin* style creates the list by binning which is an operation that scales linearly with N/P, the number of atoms per processor where N = total number of atoms and P = number of processors. It is almost always faster than the *nsq* style which scales as (N/P)^2. For unsolvated small molecules in a non-periodic box, the *nsq* choice can sometimes be faster. Either style should give the same answers.

The *multi* style is a modified binning algorithm that is useful for systems with a wide range of cutoff distances, e.g. due to different size particles. For the *bin* style, the bin size is set to 1/2 of the largest cutoff distance between any pair of atom types and a single set of bins is defined to search over for all atom types. This can be inefficient if one pair of types has a very long cutoff, but other type pairs have a much shorter cutoff. For style *multi* the bin size is set to 1/2 of the shortest cutoff distance and multiple sets of bins are defined to search over for different atom types. This imposes some extra setup overhead, but the searches themselves may be much faster for the short-cutoff cases. See the *comm_modify mode multi* command for a communication option that may also be beneficial for simulations of this kind.

The *neigh_modify* command has additional options that control how often neighbor lists are built and which pairs are stored in the list.

When a run is finished, counts of the number of neighbors stored in the pairwise list and the number of times neighbor lists were built are printed to the screen and log file. See the *Run output* doc page for details.

15.83.4 Restrictions

none

15.83.5 Related commands

neigh_modify, *units*, *comm_modify*

15.83.6 Default

0.3 bin for units = lj, skin = 0.3 sigma
2.0 bin for units = real or metal, skin = 2.0 Angstroms
0.001 bin for units = si, skin = 0.001 meters = 1.0 mm
0.1 bin for units = cgs, skin = 0.1 cm = 1.0 mm

15.84 newton command

15.84.1 Syntax

```
newton flag
newton flag1 flag2
```

- flag = *on* or *off* for both pairwise and bonded interactions
- flag1 = *on* or *off* for pairwise interactions
- flag2 = *on* or *off* for bonded interactions

15.84.2 Examples

```
newton off
newton on off
```

15.84.3 Description

This command turns Newton's 3rd law *on* or *off* for pairwise and bonded interactions. For most problems, setting Newton's 3rd law to *on* means a modest savings in computation at the cost of two times more communication. Whether this is faster depends on problem size, force cutoff lengths, a machine's compute/communication ratio, and how many processors are being used.

Setting the pairwise newton flag to *off* means that if two interacting atoms are on different processors, both processors compute their interaction and the resulting force information is not communicated. Similarly, for bonded interactions, newton *off* means that if a bond, angle, dihedral, or improper interaction contains atoms on 2 or more processors, the interaction is computed by each processor.

LAMMPS should produce the same answers for any newton flag settings, except for round-off issues.

With *run_style* *respa* and only bonded interactions (bond, angle, etc) computed in the innermost timestep, it may be faster to turn newton *off* for bonded interactions, to avoid extra communication in the innermost loop.

15.84.4 Restrictions

The newton bond setting cannot be changed after the simulation box is defined by a *read_data* or *create_box* command.

15.84.5 Related commands

run_style respa

15.84.6 Default

```
newton on
```

15.85 next command

15.85.1 Syntax

```
next variables
```

- variables = one or more variable names

15.85.2 Examples

```
next x
next a t x myTemp
```

15.85.3 Description

This command is used with variables defined by the *variable* command. It assigns the next value to the variable from the list of values defined for that variable by the *variable* command. Thus when that variable is subsequently substituted for in an input script command, the new value is used.

See the *variable* command for info on how to define and use different kinds of variables in LAMMPS input scripts. If a variable name is a single lower-case character from "a" to "z", it can be used in an input script command as $a or $z. If it is multiple letters, it can be used as ${myTemp}.

If multiple variables are used as arguments to the *next* command, then all must be of the same variable style: *index*, *loop*, *file*, *universe*, or *uloop*. An exception is that *universe*- and *uloop*-style variables can be mixed in the same *next* command.

All the variables specified with the next command are incremented by one value from their respective list of values. A *file*-style variable reads the next line from its associated file. An *atomfile*-style variable reads the next set of lines (one per atom) from its associated file. *String*- or *atom*- or *equal*- or *world*-style variables cannot be used with the next command, since they only store a single value.

When any of the variables in the next command has no more values, a flag is set that causes the input script to skip the next *jump* command encountered. This enables a loop containing a next command to exit. As explained in the *variable* command, the variable that has exhausted its values is also deleted. This allows it to be used and re-defined later in the input script. *File*-style and *atomfile*-style variables are exhausted when the end-of-file is reached.

When the next command is used with *index*- or *loop*-style variables, the next value is assigned to the variable for all processors. When the next command is used with *file*-style variables, the next line is read from its file and the string assigned to the variable. When the next command is used with *atomfile*-style variables, the next set of per-atom values is read from its file and assigned to the variable.

When the next command is used with *universe*- or *uloop*-style variables, all *universe*- or *uloop*-style variables must be listed in the next command. This is because of the manner in which the incrementing is done, using a single lock file for all variables. The next value (for each variable) is assigned to whichever processor partition executes the command first. All processors in the partition are assigned the same value(s). Running LAMMPS on multiple partitions of processors via the *-partition command-line switch*. *Universe*- and *uloop*-style variables are incremented using the files "tmp.lammps.variable" and "tmp.lammps.variable.lock" which you will see in your directory during and after such a LAMMPS run.

Here is an example of running a series of simulations using the next command with an *index*-style variable. If this input script is named in.polymer, 8 simulations would be run using data files from directories run1 through run8.

```
variable d index run1 run2 run3 run4 run5 run6 run7 run8
shell cd $d
read_data data.polymer
run 10000
shell cd ..
clear
next d
jump in.polymer
```

If the variable "d" were of style *universe*, and the same in.polymer input script were run on 3 partitions of processors, then the first 3 simulations would begin, one on each set of processors. Whichever partition finished first, it would assign variable "d" the 4th value and run another simulation, and so forth until all 8 simulations were finished.

Jump and next commands can also be nested to enable multi-level loops. For example, this script will run 15 simulations in a double loop.

```
variable i loop 3
  variable j loop 5
  clear
  ...
  read_data data.polymer.$i$j
  print Running simulation $i.$j
  run 10000
  next j
  jump in.script
next i
jump in.script
```

Here is an example of a double loop which uses the *if* and *jump* commands to break out of the inner loop when a condition is met, then continues iterating through the outer loop.

```
label       loopa
variable    a loop 5
  label     loopb
  variable  b loop 5
  print     "A,B = $a,$b"
  run       10000
```

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```
  if        $b > 2 then "jump in.script break"
  next      b
  jump      in.script loopb
label       break
variable    b delete

next        a
jump        in.script loopa
```

15.85.4 Restrictions

As described above.

15.85.5 Related commands

jump, *include*, *shell*, *variable*,

Default: none

15.86 package command

15.86.1 Syntax

```
package style args
```

- style = *gpu* or *intel* or *kokkos* or *omp*
- args = arguments specific to the style

```
gpu args = Ngpu keyword value ...
  Ngpu = # of GPUs per node
  zero or more keyword/value pairs may be appended
  keywords = neigh or newton or binsize or split or gpuID or tpa or␣
↪device or blocksize
    neigh value = yes or no
      yes = neighbor list build on GPU (default)
      no = neighbor list build on CPU
    newton = off or on
      off = set Newton pairwise flag off (default and required)
      on = set Newton pairwise flag on (currently not allowed)
    binsize value = size
      size = bin size for neighbor list construction (distance units)
    split = fraction
      fraction = fraction of atoms assigned to GPU (default = 1.0)
    gpuID values = first last
      first = ID of first GPU to be used on each node
      last = ID of last GPU to be used on each node
    tpa value = Nthreads
      Nthreads = # of GPU threads used per atom
    device value = device_type or platform_id:device_type or platform_
↪id:custom,val1,val2,val3,..,val13
```

```
      platform_id = numerical OpenCL platform id (default: -1)
      device_type = kepler or fermi or cypress or intel or phi or generic␣
↪or custom
      val1,val2,... = custom OpenCL tune parameters (see below for␣
↪details)
    blocksize value = size
      size = thread block size for pair force computation
intel args = NPhi keyword value ...
  Nphi = # of co-processors per node
  zero or more keyword/value pairs may be appended
  keywords = mode or omp or lrt or balance or ghost or tpc or tptask or␣
↪no_affinity
    mode value = single or mixed or double
      single = perform force calculations in single precision
      mixed = perform force calculations in mixed precision
      double = perform force calculations in double precision
    omp value = Nthreads
      Nthreads = number of OpenMP threads to use on CPU (default = 0)
    lrt value = yes or no
      yes = use additional thread dedicated for some PPPM calculations
      no = do not dedicate an extra thread for some PPPM calculations
    balance value = split
      split = fraction of work to offload to co-processor, -1 for dynamic
    ghost value = yes or no
      yes = include ghost atoms for offload
      no = do not include ghost atoms for offload
    tpc value = Ntpc
      Ntpc = max number of co-processor threads per co-processor core␣
↪(default = 4)
    tptask value = Ntptask
      Ntptask = max number of co-processor threads per MPI task (default␣
↪= 240)
    no_affinity values = none
kokkos args = keyword value ...
  zero or more keyword/value pairs may be appended
  keywords = neigh or neigh/qeq or neigh/thread or newton or binsize or␣
↪comm or comm/exchange or comm/forward or comm/reverse or cuda/aware
    neigh value = full or half
      full = full neighbor list
      half = half neighbor list built in thread-safe manner
    neigh/qeq value = full or half
      full = full neighbor list
      half = half neighbor list built in thread-safe manner
    neigh/thread value = off or on
      off = thread only over atoms
      on = thread over both atoms and neighbors
    newton = off or on
      off = set Newton pairwise and bonded flags off
      on = set Newton pairwise and bonded flags on
    binsize value = size
      size = bin size for neighbor list construction (distance units)
    comm value = no or host or device
      use value for comm/exchange and comm/forward and comm/reverse
    comm/exchange value = no or host or device
```

```
      comm/forward value = no or host or device
      comm/reverse value = no or host or device
        no = perform communication pack/unpack in non-KOKKOS mode
        host = perform pack/unpack on host (e.g. with OpenMP threading)
        device = perform pack/unpack on device (e.g. on GPU)
      cuda/aware = off or on
        off = do not use CUDA-aware MPI
        on = use CUDA-aware MPI (default)
  omp args = Nthreads keyword value ...
    Nthread = # of OpenMP threads to associate with each MPI process
    zero or more keyword/value pairs may be appended
    keywords = neigh
      neigh value = yes or no
        yes = threaded neighbor list build (default)
        no = non-threaded neighbor list build
```

15.86.2 Examples

```
package gpu 1
package gpu 1 split 0.75
package gpu 2 split -1.0
package gpu 1 device kepler
package gpu 1 device 2:generic
package gpu 1 device custom,32,4,8,256,11,128,256,128,32,64,8,128,128
package kokkos neigh half comm device
package omp 0 neigh no
package omp 4
package intel 1
package intel 2 omp 4 mode mixed balance 0.5
```

15.86.3 Description

This command invokes package-specific settings for the various accelerator packages available in LAMMPS. Currently the following packages use settings from this command: GPU, USER-INTEL, KOKKOS, and USER-OMP.

If this command is specified in an input script, it must be near the top of the script, before the simulation box has been defined. This is because it specifies settings that the accelerator packages use in their initialization, before a simulation is defined.

This command can also be specified from the command-line when launching LAMMPS, using the "-pk" *command-line switch*. The syntax is exactly the same as when used in an input script.

Note that all of the accelerator packages require the package command to be specified (except the OPT package), if the package is to be used in a simulation (LAMMPS can be built with an accelerator package without using it in a particular simulation). However, in all cases, a default version of the command is typically invoked by other accelerator settings.

The KOKKOS package requires a "-k on" *command-line switch* respectively, which invokes a "package kokkos" command with default settings.

For the GPU, USER-INTEL, and USER-OMP packages, if a "-sf gpu" or "-sf intel" or "-sf omp" *command-line switch* is used to auto-append accelerator suffixes to various styles in the input script, then those switches also invoke a "package gpu", "package intel", or "package omp" command with default settings.

Note: A package command for a particular style can be invoked multiple times when a simulation is setup, e.g. by the *-c on, -k on, -sf, and -pk command-line switches*, and by using this command in an input script. Each time it is used all of the style options are set, either to default values or to specified settings. I.e. settings from previous invocations do not persist across multiple invocations.

See the *Speed packages* doc page for more details about using the various accelerator packages for speeding up LAMMPS simulations.

The *gpu* style invokes settings associated with the use of the GPU package.

The *Ngpu* argument sets the number of GPUs per node. There must be at least as many MPI tasks per node as GPUs, as set by the mpirun or mpiexec command. If there are more MPI tasks (per node) than GPUs, multiple MPI tasks will share each GPU.

Optional keyword/value pairs can also be specified. Each has a default value as listed below.

The *neigh* keyword specifies where neighbor lists for pair style computation will be built. If *neigh* is *yes*, which is the default, neighbor list building is performed on the GPU. If *neigh* is *no*, neighbor list building is performed on the CPU. GPU neighbor list building currently cannot be used with a triclinic box. GPU neighbor lists are not compatible with commands that are not GPU-enabled. When a non-GPU enabled command requires a neighbor list, it will also be built on the CPU. In these cases, it will typically be more efficient to only use CPU neighbor list builds.

The *newton* keyword sets the Newton flags for pairwise (not bonded) interactions to *off* or *on*, the same as the *newton* command allows. Currently, only an *off* value is allowed, since all the GPU package pair styles require this setting. This means more computation is done, but less communication. In the future a value of *on* may be allowed, so the *newton* keyword is included as an option for compatibility with the package command for other accelerator styles. Note that the newton setting for bonded interactions is not affected by this keyword.

The *binsize* keyword sets the size of bins used to bin atoms in neighbor list builds performed on the GPU, if *neigh* = *yes* is set. If *binsize* is set to 0.0 (the default), then bins = the size of the pairwise cutoff + neighbor skin distance. This is 2x larger than the LAMMPS default used for neighbor list building on the CPU. This will be close to optimal for the GPU, so you do not normally need to use this keyword. Note that if you use a longer-than-usual pairwise cutoff, e.g. to allow for a smaller fraction of KSpace work with a *long-range Coulombic solver* because the GPU is faster at performing pairwise interactions, then it may be optimal to make the *binsize* smaller than the default. For example, with a cutoff of 20*sigma in LJ *units* and a neighbor skin distance of sigma, a *binsize* = 5.25*sigma can be more efficient than the default.

The *split* keyword can be used for load balancing force calculations between CPU and GPU cores in GPU-enabled pair styles. If 0 < *split* < 1.0, a fixed fraction of particles is offloaded to the GPU while force calculation for the other particles occurs simultaneously on the CPU. If *split* < 0.0, the optimal fraction (based on CPU and GPU timings) is calculated every 25 timesteps, i.e. dynamic load-balancing across the CPU and GPU is performed. If *split* = 1.0, all force calculations for GPU accelerated pair styles are performed on the GPU. In this case, other *hybrid* pair interactions, *bond*, *angle*, *dihedral*, *improper*, and *long-range* calculations can be performed on the CPU while the GPU is performing force calculations for the GPU-enabled pair style. If all CPU force computations complete before the GPU completes, LAMMPS will block until the GPU has finished before continuing the timestep.

As an example, if you have two GPUs per node and 8 CPU cores per node, and would like to run on 4 nodes (32 cores) with dynamic balancing of force calculation across CPU and GPU cores, you could specify

```
mpirun -np 32 -sf gpu -in in.script     # launch command
package gpu 2 split -1                  # input script command
```

In this case, all CPU cores and GPU devices on the nodes would be utilized. Each GPU device would be shared by 4 CPU cores. The CPU cores would perform force calculations for some fraction of the particles at the same time the GPUs performed force calculation for the other particles.

The *gpuID* keyword allows selection of which GPUs on each node will be used for a simulation. The *first* and *last* values specify the GPU IDs to use (from 0 to Ngpu-1). By default, first = 0 and last = Ngpu-1, so that all GPUs are used, assuming Ngpu is set to the number of physical GPUs. If you only wish to use a subset, set Ngpu to a smaller number and first/last to a sub-range of the available GPUs.

The *tpa* keyword sets the number of GPU thread per atom used to perform force calculations. With a default value of 1, the number of threads will be chosen based on the pair style, however, the value can be set explicitly with this keyword to fine-tune performance. For large cutoffs or with a small number of particles per GPU, increasing the value can improve performance. The number of threads per atom must be a power of 2 and currently cannot be greater than 32.

The *device* keyword can be used to tune parameters optimized for a specific accelerator and platform when using OpenCL. OpenCL supports the concept of a **platform**, which represents one or more devices that share the same driver (e.g. there would be a different platform for GPUs from different vendors or for CPU based accelerator support). In LAMMPS only one platform can be active at a time and by default the first platform with an accelerator is selected. This is equivalent to using a platform ID of -1. The platform ID is a number corresponding to the output of the ocl_get_devices tool. The platform ID is passed to the GPU library, by prefixing the *device* keyword with that number separated by a colon. For CUDA, the *device* keyword is ignored. Currently, the device tuning support is limited to NVIDIA Kepler, NVIDIA Fermi, AMD Cypress, Intel x86_64 CPU, Intel Xeon Phi, or a generic device. More devices may be added later. The default device type can be specified when building LAMMPS with the GPU library, via setting a variable in the lib/gpu/Makefile that is used.

In addition, a device type *custom* is available, which is followed by 13 comma separated numbers, which allows to set those tweakable parameters from the package command. It can be combined with the (colon separated) platform id. The individual settings are:

- MEM_THREADS
- THREADS_PER_ATOM
- THREADS_PER_CHARGE
- BLOCK_PAIR
- MAX_SHARED_TYPES
- BLOCK_NBOR_BUILD
- BLOCK_BIO_PAIR
- BLOCK_ELLIPSE
- WARP_SIZE
- PPPM_BLOCK_1D
- BLOCK_CELL_2D
- BLOCK_CELL_ID
- MAX_BIO_SHARED_TYPES

The *blocksize* keyword allows you to tweak the number of threads used per thread block. This number should be a multiple of 32 (for GPUs) and its maximum depends on the specific GPU hardware. Typical choices are 64, 128, or 256. A larger block size increases occupancy of individual GPU cores, but reduces the total number of thread blocks, thus may lead to load imbalance.

The *intel* style invokes settings associated with the use of the USER-INTEL package. All of its settings, except the *omp* and *mode* keywords, are ignored if LAMMPS was not built with Xeon Phi co-processor support. All of its settings, including the *omp* and *mode* keyword are applicable if LAMMPS was built with co-processor support.

The *Nphi* argument sets the number of co-processors per node. This can be set to any value, including 0, if LAMMPS was not built with co-processor support.

Optional keyword/value pairs can also be specified. Each has a default value as listed below.

The *omp* keyword determines the number of OpenMP threads allocated for each MPI task when any portion of the interactions computed by a USER-INTEL pair style are run on the CPU. This can be the case even if LAMMPS was built with co-processor support; see the *balance* keyword discussion below. If you are running with less MPI tasks/node than there are CPUs, it can be advantageous to use OpenMP threading on the CPUs.

Note: The *omp* keyword has nothing to do with co-processor threads on the Xeon Phi; see the *tpc* and *tptask* keywords below for a discussion of co-processor threads.

The *Nthread* value for the *omp* keyword sets the number of OpenMP threads allocated for each MPI task. Setting *Nthread* = 0 (the default) instructs LAMMPS to use whatever value is the default for the given OpenMP environment. This is usually determined via the *OMP_NUM_THREADS* environment variable or the compiler runtime, which is usually a value of 1.

For more details, including examples of how to set the OMP_NUM_THREADS environment variable, see the discussion of the *Nthreads* setting on this doc page for the "package omp" command. Nthreads is a required argument for the USER-OMP package. Its meaning is exactly the same for the USER-INTEL package.

Note: If you build LAMMPS with both the USER-INTEL and USER-OMP packages, be aware that both packages allow setting of the *Nthreads* value via their package commands, but there is only a single global *Nthreads* value used by OpenMP. Thus if both package commands are invoked, you should insure the two values are consistent. If they are not, the last one invoked will take precedence, for both packages. Also note that if the *-sf hybrid intel omp command-line switch* is used, it invokes a "package intel" command, followed by a "package omp" command, both with a setting of *Nthreads* = 0.

The *mode* keyword determines the precision mode to use for computing pair style forces, either on the CPU or on the co-processor, when using a USER-INTEL supported *pair style*. It can take a value of *single*, *mixed* which is the default, or *double*. *Single* means single precision is used for the entire force calculation. *Mixed* means forces between a pair of atoms are computed in single precision, but accumulated and stored in double precision, including storage of forces, torques, energies, and virial quantities. *Double* means double precision is used for the entire force calculation.

The *lrt* keyword can be used to enable "Long Range Thread (LRT)" mode. It can take a value of *yes* to enable and *no* to disable. LRT mode generates an extra thread (in addition to any OpenMP threads specified with the OMP_NUM_THREADS environment variable or the *omp* keyword). The extra thread is dedicated for performing part of the *PPPM solver* computations and communications. This can improve parallel performance on processors supporting Simultaneous Multithreading (SMT) such as Hyper-Threading (HT) on Intel processors. In this mode, one additional thread is generated per MPI process. LAMMPS will generate a warning in the case that more threads are used than available in SMT hardware on a node. If the PPPM solver from the USER-INTEL package is not used, then the LRT setting is ignored and no extra threads are generated. Enabling LRT will replace the *run_style* with the *verlet/lrt/intel* style that is identical to the default *verlet* style aside from supporting the LRT feature. This feature requires setting the pre-processor flag -DLMP_INTEL_USELRT in the makefile when compiling LAMMPS.

The *balance* keyword sets the fraction of *pair style* work offloaded to the co-processor for split values between 0.0 and 1.0 inclusive. While this fraction of work is running on the co-processor, other calculations will run on the host, including neighbor and pair calculations that are not offloaded, as well as angle, bond, dihedral, kspace, and some MPI communications. If *split* is set to -1, the fraction of work is dynamically adjusted automatically throughout the run. This typically give performance within 5 to 10 percent of the optimal fixed fraction.

The *ghost* keyword determines whether or not ghost atoms, i.e. atoms at the boundaries of processor sub-domains, are offloaded for neighbor and force calculations. When the value = "no", ghost atoms are not offloaded. This option can reduce the amount of data transfer with the co-processor and can also overlap MPI communication of forces with

computation on the co-processor when the *newton pair* setting is "on". When the value = "yes", ghost atoms are offloaded. In some cases this can provide better performance, especially if the *balance* fraction is high.

The *tpc* keyword sets the max # of co-processor threads *Ntpc* that will run on each core of the co-processor. The default value = 4, which is the number of hardware threads per core supported by the current generation Xeon Phi chips.

The *tptask* keyword sets the max # of co-processor threads (Ntptask* assigned to each MPI task. The default value = 240, which is the total # of threads an entire current generation Xeon Phi chip can run (240 = 60 cores * 4 threads/core). This means each MPI task assigned to the Phi will enough threads for the chip to run the max allowed, even if only 1 MPI task is assigned. If 8 MPI tasks are assigned to the Phi, each will run with 30 threads. If you wish to limit the number of threads per MPI task, set *tptask* to a smaller value. E.g. for *tptask* = 16, if 8 MPI tasks are assigned, each will run with 16 threads, for a total of 128.

Note that the default settings for *tpc* and *tptask* are fine for most problems, regardless of how many MPI tasks you assign to a Phi.

The *no_affinity* keyword will turn off automatic setting of core affinity for MPI tasks and OpenMP threads on the host when using offload to a co-processor. Affinity settings are used when possible to prevent MPI tasks and OpenMP threads from being on separate NUMA domains and to prevent offload threads from interfering with other processes/threads used for LAMMPS.

The *kokkos* style invokes settings associated with the use of the KOKKOS package.

All of the settings are optional keyword/value pairs. Each has a default value as listed below.

The *neigh* keyword determines how neighbor lists are built. A value of *half* uses a thread-safe variant of half-neighbor lists, the same as used by most pair styles in LAMMPS, which is the default when running on CPUs (i.e. the Kokkos CUDA back end is not enabled).

A value of *full* uses a full neighbor lists and is the default when running on GPUs. This performs twice as much computation as the *half* option, however that is often a win because it is thread-safe and doesn't require atomic operations in the calculation of pair forces. For that reason, *full* is the default setting for GPUs. However, when running on CPUs, a *half* neighbor list is the default because it are often faster, just as it is for non-accelerated pair styles. Similarly, the *neigh/qeq* keyword determines how neighbor lists are built for *fix qeq/reax/kk*. If not explicitly set, the value of *neigh/qeq* will match *neigh*.

If the *neigh/thread* keyword is set to *off*, then the KOKKOS package threads only over atoms. However, for small systems, this may not expose enough parallelism to keep a GPU busy. When this keyword is set to *on*, the KOKKOS package threads over both atoms and neighbors of atoms. When using *neigh/thread on*, a full neighbor list must also be used. Using *neigh/thread on* may be slower for large systems, so this this option is turned on by default only when there are 16K atoms or less owned by an MPI rank and when using a full neighbor list. Not all KOKKOS-enabled potentials support this keyword yet, and only thread over atoms. Many simple pair-wise potentials such as Lennard-Jones do support threading over both atoms and neighbors.

The *newton* keyword sets the Newton flags for pairwise and bonded interactions to *off* or *on*, the same as the *newton* command allows. The default for GPUs is *off* because this will almost always give better performance for the KOKKOS package. This means more computation is done, but less communication. However, when running on CPUs a value of *on* is the default since it can often be faster, just as it is for non-accelerated pair styles

The *binsize* keyword sets the size of bins used to bin atoms in neighbor list builds. The same value can be set by the *neigh_modify binsize* command. Making it an option in the package kokkos command allows it to be set from the command line. The default value for CPUs is 0.0, which means the LAMMPS default will be used, which is bins = 1/2 the size of the pairwise cutoff + neighbor skin distance. This is fine when neighbor lists are built on the CPU. For GPU builds, a 2x larger binsize equal to the pairwise cutoff + neighbor skin is often faster, which is the default. Note that if you use a longer-than-usual pairwise cutoff, e.g. to allow for a smaller fraction of KSpace work with a *long-range Coulombic solver* because the GPU is faster at performing pairwise interactions, then this rule of thumb may give too large a binsize and the default should be overridden with a smaller value.

The *comm* and *comm/exchange* and *comm/forward* and *comm/reverse* keywords determine whether the host or device performs the packing and unpacking of data when communicating per-atom data between processors. "Exchange" communication happens only on timesteps that neighbor lists are rebuilt. The data is only for atoms that migrate to new processors. "Forward" communication happens every timestep. "Reverse" communication happens every timestep if the *newton* option is on. The data is for atom coordinates and any other atom properties that needs to be updated for ghost atoms owned by each processor.

The *comm* keyword is simply a short-cut to set the same value for both the *comm/exchange* and *comm/forward* and *comm/reverse* keywords.

The value options for all 3 keywords are *no* or *host* or *device*. A value of *no* means to use the standard non-KOKKOS method of packing/unpacking data for the communication. A value of *host* means to use the host, typically a multi-core CPU, and perform the packing/unpacking in parallel with threads. A value of *device* means to use the device, typically a GPU, to perform the packing/unpacking operation.

The optimal choice for these keywords depends on the input script and the hardware used. The *no* value is useful for verifying that the Kokkos-based *host* and *device* values are working correctly. It is the default when running on CPUs since it is usually the fastest.

When running on CPUs or Xeon Phi, the *host* and *device* values work identically. When using GPUs, the *device* value is the default since it will typically be optimal if all of your styles used in your input script are supported by the KOKKOS package. In this case data can stay on the GPU for many timesteps without being moved between the host and GPU, if you use the *device* value. If your script uses styles (e.g. fixes) which are not yet supported by the KOKKOS package, then data has to be move between the host and device anyway, so it is typically faster to let the host handle communication, by using the *host* value. Using *host* instead of *no* will enable use of multiple threads to pack/unpack communicated data. When running small systems on a GPU, performing the exchange pack/unpack on the host CPU can give speedup since it reduces the number of CUDA kernel launches.

The *cuda/aware* keyword chooses whether CUDA-aware MPI will be used. When this keyword is set to *on*, buffers in GPU memory are passed directly through MPI send/receive calls. This reduces overhead of first copying the data to the host CPU. However CUDA-aware MPI is not supported on all systems, which can lead to segmentation faults and would require using a value of *off*. If LAMMPS can safely detect that CUDA-aware MPI is not available (currently only possible with OpenMPI v2.0.0 or later), then the *cuda/aware* keyword is automatically set to *off* by default. When the *cuda/aware* keyword is set to *off* while any of the *comm* keywords are set to *device*, the value for these *comm* keywords will be automatically changed to *host*. This setting has no effect if not running on GPUs or if using only one MPI rank. CUDA-aware MPI is available for OpenMPI 1.8 (or later versions), Mvapich2 1.9 (or later) when the "MV2_USE_CUDA" environment variable is set to "1", CrayMPI, and IBM Spectrum MPI when the "-gpu" flag is used.

The *omp* style invokes settings associated with the use of the USER-OMP package.

The *Nthread* argument sets the number of OpenMP threads allocated for each MPI task. For example, if your system has nodes with dual quad-core processors, it has a total of 8 cores per node. You could use two MPI tasks per node (e.g. using the -ppn option of the mpirun command in MPICH or -npernode in OpenMPI), and set *Nthreads* = 4. This would use all 8 cores on each node. Note that the product of MPI tasks * threads/task should not exceed the physical number of cores (on a node), otherwise performance will suffer.

Setting *Nthread* = 0 instructs LAMMPS to use whatever value is the default for the given OpenMP environment. This is usually determined via the *OMP_NUM_THREADS* environment variable or the compiler runtime. Note that in most cases the default for OpenMP capable compilers is to use one thread for each available CPU core when *OMP_NUM_THREADS* is not explicitly set, which can lead to poor performance.

Here are examples of how to set the environment variable when launching LAMMPS:

```
env OMP_NUM_THREADS=4 lmp_machine -sf omp -in in.script
env OMP_NUM_THREADS=2 mpirun -np 2 lmp_machine -sf omp -in in.script
mpirun -x OMP_NUM_THREADS=2 -np 2 lmp_machine -sf omp -in in.script
```

or you can set it permanently in your shell's start-up script. All three of these examples use a total of 4 CPU cores.

Note that different MPI implementations have different ways of passing the OMP_NUM_THREADS environment variable to all MPI processes. The 2nd example line above is for MPICH; the 3rd example line with -x is for OpenMPI. Check your MPI documentation for additional details.

What combination of threads and MPI tasks gives the best performance is difficult to predict and can depend on many components of your input. Not all features of LAMMPS support OpenMP threading via the USER-OMP package and the parallel efficiency can be very different, too.

Optional keyword/value pairs can also be specified. Each has a default value as listed below.

The *neigh* keyword specifies whether neighbor list building will be multi-threaded in addition to force calculations. If *neigh* is set to *no* then neighbor list calculation is performed only by MPI tasks with no OpenMP threading. If *mode* is *yes* (the default), a multi-threaded neighbor list build is used. Using *neigh* = *yes* is almost always faster and should produce identical neighbor lists at the expense of using more memory. Specifically, neighbor list pages are allocated for all threads at the same time and each thread works within its own pages.

15.86.4 Restrictions

This command cannot be used after the simulation box is defined by a *read_data* or *create_box* command.

The gpu style of this command can only be invoked if LAMMPS was built with the GPU package. See the *Build package* doc page for more info.

The intel style of this command can only be invoked if LAMMPS was built with the USER-INTEL package. See the *Build package* doc page for more info.

The kk style of this command can only be invoked if LAMMPS was built with the KOKKOS package. See the *Build package* doc page for more info.

The omp style of this command can only be invoked if LAMMPS was built with the USER-OMP package. See the *Build package* doc page for more info.

15.86.5 Related commands

suffix, *-pk command-line switch*

15.86.6 Default

For the GPU package, the default is Ngpu = 1 and the option defaults are neigh = yes, newton = off, binsize = 0.0, split = 1.0, gpuID = 0 to Ngpu-1, tpa = 1, and device = not used. These settings are made automatically if the "-sf gpu" *command-line switch* is used. If it is not used, you must invoke the package gpu command in your input script or via the "-pk gpu" *command-line switch*.

For the USER-INTEL package, the default is Nphi = 1 and the option defaults are omp = 0, mode = mixed, lrt = no, balance = -1, tpc = 4, tptask = 240. The default ghost option is determined by the pair style being used. This value is output to the screen in the offload report at the end of each run. Note that all of these settings, except "omp" and "mode", are ignored if LAMMPS was not built with Xeon Phi co-processor support. These settings are made automatically if the "-sf intel" *command-line switch* is used. If it is not used, you must invoke the package intel command in your input script or via the "-pk intel" *command-line switch*.

For the KOKKOS package, the option defaults for GPUs are neigh = full, neigh/qeq = full, newton = off, binsize for GPUs = 2x LAMMPS default value, comm = device, cuda/aware = on. When LAMMPS can safely detect that CUDA-aware MPI is not available, the default value of cuda/aware becomes "off". For CPUs or Xeon Phis, the option

defaults are neigh = half, neigh/qeq = half, newton = on, binsize = 0.0, and comm = no. The option neigh/thread = on when there are 16K atoms or less on an MPI rank, otherwise it is "off". These settings are made automatically by the required "-k on" *command-line switch*. You can change them by using the package kokkos command in your input script or via the *-pk kokkos command-line switch*.

For the OMP package, the default is Nthreads = 0 and the option defaults are neigh = yes. These settings are made automatically if the "-sf omp" *command-line switch* is used. If it is not used, you must invoke the package omp command in your input script or via the "-pk omp" *command-line switch*.

15.87 pair_coeff command

15.87.1 Syntax

```
pair_coeff I J args
```

- I,J = atom types (see asterisk form below)
- args = coefficients for one or more pairs of atom types

15.87.2 Examples

```
pair_coeff 1 2 1.0 1.0 2.5
pair_coeff 2 \* 1.0 1.0
pair_coeff 3\* 1\*2 1.0 1.0 2.5
pair_coeff \* \* 1.0 1.0
pair_coeff \* \* nialhjea 1 1 2
pair_coeff \* 3 morse.table ENTRY1
pair_coeff 1 2 lj/cut 1.0 1.0 2.5 (for pair_style hybrid)
```

15.87.3 Description

Specify the pairwise force field coefficients for one or more pairs of atom types. The number and meaning of the coefficients depends on the pair style. Pair coefficients can also be set in the data file read by the *read_data* command or in a restart file.

I and J can be specified in one of two ways. Explicit numeric values can be used for each, as in the 1st example above. I <= J is required. LAMMPS sets the coefficients for the symmetric J,I interaction to the same values.

A wildcard asterisk can be used in place of or in conjunction with the I,J arguments to set the coefficients for multiple pairs of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). Note that only type pairs with I <= J are considered; if asterisks imply type pairs where J < I, they are ignored.

Note that a pair_coeff command can override a previous setting for the same I,J pair. For example, these commands set the coeffs for all I,J pairs, then overwrite the coeffs for just the I,J = 2,3 pair:

```
pair_coeff \* \* 1.0 1.0 2.5
pair_coeff 2 3 2.0 1.0 1.12
```

A line in a data file that specifies pair coefficients uses the exact same format as the arguments of the pair_coeff command in an input script, with the exception of the I,J type arguments. In each line of the "Pair Coeffs" section of a data file, only a single type I is specified, which sets the coefficients for type I interacting with type I. This is because

the section has exactly N lines, where N = the number of atom types. For this reason, the wild-card asterisk should also not be used as part of the I argument. Thus in a data file, the line corresponding to the 1st example above would be listed as

```
2 1.0 1.0 2.5
```

For many potentials, if coefficients for type pairs with I != J are not set explicitly by a pair_coeff command, the values are inferred from the I,I and J,J settings by mixing rules; see the *pair_modify* command for a discussion. Details on this option as it pertains to individual potentials are described on the doc page for the potential.

Many pair styles, typically for many-body potentials, use tabulated potential files as input, when specifying the pair_coeff command. Potential files provided with LAMMPS are in the potentials directory of the distribution. For some potentials, such as EAM, other archives of suitable files can be found on the Web. They can be used with LAMMPS so long as they are in the format LAMMPS expects, as discussed on the individual doc pages.

When a pair_coeff command using a potential file is specified, LAMMPS looks for the potential file in 2 places. First it looks in the location specified. E.g. if the file is specified as "niu3.eam", it is looked for in the current working directory. If it is specified as "../potentials/niu3.eam", then it is looked for in the potentials directory, assuming it is a sister directory of the current working directory. If the file is not found, it is then looked for in the directory specified by the LAMMPS_POTENTIALS environment variable. Thus if this is set to the potentials directory in the LAMMPS distribution, then you can use those files from anywhere on your system, without copying them into your working directory. Environment variables are set in different ways for different shells. Here are example settings for

csh, tcsh:

```
% setenv LAMMPS_POTENTIALS /path/to/lammps/potentials
```

bash:

```
% export LAMMPS_POTENTIALS=/path/to/lammps/potentials
```

Windows:

```
% set LAMMPS_POTENTIALS="C:\Path to LAMMPS\Potentials"
```

The alphabetic list of pair styles defined in LAMMPS is given on the *pair_style* doc page. They are also listed in more compact form on the *Commands pair* doc page.

Click on the style to display the formula it computes and its coefficients as specified by the associated pair_coeff command.

15.87.4 Restrictions

This command must come after the simulation box is defined by a *read_data*, *read_restart*, or *create_box* command.

15.87.5 Related commands

pair_style, *pair_modify*, *read_data*, *read_restart*, *pair_write*

Default: none

15.88 pair_modify command

15.88.1 Syntax

```
pair_modify keyword values ...
```

- one or more keyword/value pairs may be listed
- keyword = *pair* or *shift* or *mix* or *table* or *table/disp* or *tabinner* or *tabinner/disp* or *tail* or *compute* or *nofdotr* or *special* or *compute/tally*

```
pair value = sub-style N
  sub-style = sub-style of pair hybrid
  N = which instance of sub-style (1 to M), only specify if sub-style is␣
↪used multiple times
mix value = geometric or arithmetic or sixthpower
shift value = yes or no
table value = N
  2^N = # of values in table
table/disp value = N
  2^N = # of values in table
tabinner value = cutoff
  cutoff = inner cutoff at which to begin table (distance units)
tabinner/disp value = cutoff
  cutoff = inner cutoff at which to begin table (distance units)
tail value = yes or no
compute value = yes or no
nofdotr value = none
special values = which wt1 wt2 wt3
   which = lj/coul or lj or coul
   w1,w2,w3 = 1-2, 1-3, 1-4 weights from 0.0 to 1.0 inclusive
compute/tally value = yes or no
```

15.88.2 Examples

```
pair_modify shift yes mix geometric
pair_modify tail yes
pair_modify table 12
pair_modify pair lj/cut compute no
pair_modify pair tersoff compute/tally no
pair_modify pair lj/cut/coul/long 1 special lj/coul 0.0 0.0 0.0
pair_modify pair lj/cut/coul/long special lj 0.0 0.0 0.5 special coul 0.0 0.0 0.
↪8333333
```

15.88.3 Description

Modify the parameters of the currently defined pair style. If the pair style is *hybrid or hybrid/overlay*, then the specified parameters are by default modified for all the hybrid sub-styles.

Note: The behavior for hybrid pair styles can be changed by using the *pair* keyword, which allows selection of a specific sub-style to apply all remaining keywords to. The *special* and *compute/tally* keywords can **only** be used in conjunction with the *pair* keyword. See further details about these 3 keywords below.

The *mix* keyword affects pair coefficients for interactions between atoms of type I and J, when I != J and the coefficients are not explicitly set in the input script. Note that coefficients for I = J must be set explicitly, either in the input script via the *pair_coeff* command or in the "Pair Coeffs" section of the *data file*. For some pair styles it is not necessary to specify coefficients when I != J, since a "mixing" rule will create them from the I,I and J,J settings. The pair_modify *mix* value determines what formulas are used to compute the mixed coefficients. In each case, the cutoff distance is mixed the same way as sigma.

Note that not all pair styles support mixing and some mix options are not available for certain pair styles. Also, there are additional restrictions when using *pair style hybrid or hybrid/overlay*. See the doc page for individual pair styles for those restrictions. Note also that the *pair_coeff* command also can be used to directly set coefficients for a specific I != J pairing, in which case no mixing is performed.

- mix *geometric*

$$\epsilon_{ij} = \sqrt{\epsilon_i \epsilon_j}$$
$$\sigma_{ij} = \sqrt{\sigma_i \sigma_j}$$

- mix *arithmetic*

$$\epsilon_{ij} = \sqrt{\epsilon_i \epsilon_j}$$
$$\sigma_{ij} = \frac{1}{2}(\sigma_i + \sigma_j)$$

- mix *sixthpower*

$$\epsilon_{ij} = \frac{2\sqrt{\epsilon_i \epsilon_j}\sigma_i^3 \sigma_j^3}{\sigma_i^6 + \sigma_j^6}$$
$$\sigma_{ij} = \left(\frac{1}{2}(\sigma_i^6 + \sigma_j^6)\right)^{\frac{1}{6}}$$

The *shift* keyword determines whether a Lennard-Jones potential is shifted at its cutoff to 0.0. If so, this adds an energy term to each pairwise interaction which will be included in the thermodynamic output, but does not affect pair forces or atom trajectories. See the doc page for individual pair styles to see which ones support this option.

The *table* and *table/disp* keywords apply to pair styles with a long-range Coulombic term or long-range dispersion term respectively; see the doc page for individual styles to see which potentials support these options. If N is non-zero, a table of length 2^N is pre-computed for forces and energies, which can shrink their computational cost by up to a factor of 2. The table is indexed via a bit-mapping technique *(Wolff)* and a linear interpolation is performed between adjacent table values. In our experiments with different table styles (lookup, linear, spline), this method typically gave the best performance in terms of speed and accuracy.

The choice of table length is a tradeoff in accuracy versus speed. A larger N yields more accurate force computations, but requires more memory which can slow down the computation due to cache misses. A reasonable value of N is between 8 and 16. The default value of 12 (table of length 4096) gives approximately the same accuracy as the no-table (N = 0) option. For N = 0, forces and energies are computed directly, using a polynomial fit for the needed erfc()

function evaluation, which is what earlier versions of LAMMPS did. Values greater than 16 typically slow down the simulation and will not improve accuracy; values from 1 to 8 give unreliable results.

The *tabinner* and *tabinner/disp* keywords set an inner cutoff above which the pairwise computation is done by table lookup (if tables are invoked), for the corresponding Coulombic and dispersion tables discussed with the *table* and *table/disp* keywords. The smaller the cutoff is set, the less accurate the table becomes (for a given number of table values), which can require use of larger tables. The default cutoff value is sqrt(2.0) distance units which means nearly all pairwise interactions are computed via table lookup for simulations with "real" units, but some close pairs may be computed directly (non-table) for simulations with "lj" units.

When the *tail* keyword is set to *yes*, certain pair styles will add a long-range VanderWaals tail "correction" to the energy and pressure. These corrections are bookkeeping terms which do not affect dynamics, unless a constant-pressure simulation is being performed. See the doc page for individual styles to see which support this option. These corrections are included in the calculation and printing of thermodynamic quantities (see the *thermo_style* command). Their effect will also be included in constant NPT or NPH simulations where the pressure influences the simulation box dimensions (e.g. the *fix npt* and *fix nph* commands). The formulas used for the long-range corrections come from equation 5 of *(Sun)*.

Note: The tail correction terms are computed at the beginning of each run, using the current atom counts of each atom type. If atoms are deleted (or lost) or created during a simulation, e.g. via the *fix gcmc* command, the correction factors are not re-computed. If you expect the counts to change dramatically, you can break a run into a series of shorter runs so that the correction factors are re-computed more frequently.

Several additional assumptions are inherent in using tail corrections, including the following:

- The simulated system is a 3d bulk homogeneous liquid. This option should not be used for systems that are non-liquid, 2d, have a slab geometry (only 2d periodic), or inhomogeneous.
- G(r), the radial distribution function (rdf), is unity beyond the cutoff, so a fairly large cutoff should be used (i.e. 2.5 sigma for an LJ fluid), and it is probably a good idea to verify this assumption by checking the rdf. The rdf is not exactly unity beyond the cutoff for each pair of interaction types, so the tail correction is necessarily an approximation.

  The tail corrections are computed at the beginning of each simulation run. If the number of atoms changes during the run, e.g. due to atoms leaving the simulation domain, or use of the *fix gcmc* command, then the corrections are not updated to reflect the changed atom count. If this is a large effect in your simulation, you should break the long run into several short runs, so that the correction factors are re-computed multiple times.
- Thermophysical properties obtained from calculations with this option enabled will not be thermodynamically consistent with the truncated force-field that was used. In other words, atoms do not feel any LJ pair interactions beyond the cutoff, but the energy and pressure reported by the simulation include an estimated contribution from those interactions.

The *compute* keyword allows pairwise computations to be turned off, even though a *pair_style* is defined. This is not useful for running a real simulation, but can be useful for debugging purposes or for performing a *rerun* simulation, when you only wish to compute partial forces that do not include the pairwise contribution.

Two examples are as follows. First, this option allows you to perform a simulation with *pair_style hybrid* with only a subset of the hybrid sub-styles enabled. Second, this option allows you to perform a simulation with only long-range interactions but no short-range pairwise interactions. Doing this by simply not defining a pair style will not work, because the *kspace_style* command requires a Kspace-compatible pair style be defined.

The *nofdotr* keyword allows to disable an optimization that computes the global stress tensor from the total forces and atom positions rather than from summing forces between individual pairs of atoms.

The *pair* keyword can only be used with the *hybrid and hybrid/overlay* pair styles. If used, it must appear first in the list of keywords.

Its meaning is that all the following parameters will only be modified for the specified sub-style. If the sub-style is defined multiple times, then an additional numeric argument *N* must also be specified, which is a number from 1 to M where M is the number of times the sub-style was listed in the *pair_style hybrid* command. The extra number indicates which instance of the sub-style the remaining keywords will be applied to.

The *special* and *compute/tally* keywords can **only** be used in conjunction with the *pair* keyword and they must directly follow it. I.e. any other keyword, must appear after *pair*, *special*, and *compute/tally*.

The *special* keyword overrides the global *special_bonds* 1-2, 1-3, 1-4 exclusion settings (weights) for the sub-style selected by the *pair* keyword.

Similar to the *special_bonds* command, it takes 4 arguments. The *which* argument can be *lj* to change only the non-Coulomb weights (e.g. Lennard-Jones or Buckingham), *coul* to change only the Coulombic settings, or *lj/coul* to change both to the same values. The *wt1,wt2,wt3* values are numeric weights from 0.0 to 1.0 inclusive, for the 1-2, 1-3, and 1-4 bond topology neighbors, respectively. The *special* keyword can be used multiple times, e.g. to set the *lj* and *coul* settings to different values.

Note: The *special* keyword is not compatible with pair styles from the GPU or the USER-INTEL package and attempting to use it will cause an error.

Note: Weights of exactly 0.0 or 1.0 in the *special_bonds* command have implications on the neighbor list construction, which means that they cannot be overridden by using the *special* keyword. One workaround for this restriction is to use the *special_bonds* command with weights like 1.0e-10 or 0.999999999 instead of 0.0 or 1.0, respectively, which enables to reset each them to any value between 0.0 and 1.0 inclusively. Otherwise you can set **all** global weights to an arbitrary number between 0.0 or 1.0, like 0.5, and then you have to override **all** *special* settings for **all** sub-styles which use the 1-2, 1-3, and 1-4 exclusion weights in their force/energy computation.

The *compute/tally* keyword disables or enables registering *compute */tally* computes for the sub-style specified by the *pair* keyword. Use *no* to disable, or *yes* to enable.

Note: The "pair_modify pair compute/tally" command must be issued **before** the corresponding compute style is defined.

15.88.4 Restrictions

You cannot use *shift* yes with *tail* yes, since those are conflicting options. You cannot use *tail* yes with 2d simulations. You cannot use *special* with pair styles from the GPU or USER-INTEL package.

15.88.5 Related commands

pair_style, *pair_style hybrid*, *pair_coeff*, *thermo_style*, *compute */tally*

15.88.6 Default

The option defaults are mix = geometric, shift = no, table = 12, tabinner = sqrt(2.0), tail = no, and compute = yes.

Note that some pair styles perform mixing, but only a certain style of mixing. See the doc pages for individual pair styles for details.

(Wolff) Wolff and Rudd, Comp Phys Comm, 120, 200-32 (1999).

(Sun) Sun, J Phys Chem B, 102, 7338-7364 (1998).

15.89 pair_style command

15.89.1 Syntax

```
pair_style style args
```

- style = one of the styles from the list below
- args = arguments used by a particular style

15.89.2 Examples

```
pair_style lj/cut 2.5
pair_style eam/alloy
pair_style hybrid lj/charmm/coul/long 10.0 eam
pair_style table linear 1000
pair_style none
```

15.89.3 Description

Set the formula(s) LAMMPS uses to compute pairwise interactions. In LAMMPS, pair potentials are defined between pairs of atoms that are within a cutoff distance and the set of active interactions typically changes over time. See the *bond_style* command to define potentials between pairs of bonded atoms, which typically remain in place for the duration of a simulation.

In LAMMPS, pairwise force fields encompass a variety of interactions, some of which include many-body effects, e.g. EAM, Stillinger-Weber, Tersoff, REBO potentials. They are still classified as "pairwise" potentials because the set of interacting atoms changes with time (unlike molecular bonds) and thus a neighbor list is used to find nearby interacting atoms.

Hybrid models where specified pairs of atom types interact via different pair potentials can be setup using the *hybrid* pair style.

The coefficients associated with a pair style are typically set for each pair of atom types, and are specified by the *pair_coeff* command or read from a file by the *read_data* or *read_restart* commands.

The *pair_modify* command sets options for mixing of type I-J interaction coefficients and adding energy offsets or tail corrections to Lennard-Jones potentials. Details on these options as they pertain to individual potentials are described on the doc page for the potential. Likewise, info on whether the potential information is stored in a *restart file* is listed on the potential doc page.

In the formulas listed for each pair style, E is the energy of a pairwise interaction between two atoms separated by a distance r. The force between the atoms is the negative derivative of this expression.

If the pair_style command has a cutoff argument, it sets global cutoffs for all pairs of atom types. The distance(s) can be smaller or larger than the dimensions of the simulation box.

Typically, the global cutoff value can be overridden for a specific pair of atom types by the *pair_coeff* command. The pair style settings (including global cutoffs) can be changed by a subsequent pair_style command using the same style. This will reset the cutoffs for all atom type pairs, including those previously set explicitly by a *pair_coeff* command. The exceptions to this are that pair_style *table* and *hybrid* settings cannot be reset. A new pair_style command for these styles will wipe out all previously specified pair_coeff values.

Here is an alphabetic list of pair styles defined in LAMMPS. They are also listed in more compact form on the *Commands pair* doc page.

Click on the style to display the formula it computes, any additional arguments specified in the pair_style command, and coefficients specified by the associated *pair_coeff* command.

There are also additional accelerated pair styles included in the LAMMPS distribution for faster performance on CPUs, GPUs, and KNLs. The individual style names on the *Commands pair* doc page are followed by one or more of (g,i,k,o,t) to indicate which accelerated styles exist.

- *none* - turn off pairwise interactions
- *hybrid* - multiple styles of pairwise interactions
- *hybrid/overlay* - multiple styles of superposed pairwise interactions
- *zero* - neighbor list but no interactions
- *adp* - angular dependent potential (ADP) of Mishin
- *agni* - machine learned potential mapping atomic environment to forces
- *airebo* - AIREBO potential of Stuart
- *airebo/morse* - AIREBO with Morse instead of LJ
- *atm* - Axilrod-Teller-Muto potential
- *awpmd/cut* - Antisymmetrized Wave Packet MD potential for atoms and electrons
- *beck* - Beck potential
- *body/nparticle* - interactions between body particles
- *body/rounded/polygon* - granular-style 2d polygon potential
- *body/rounded/polyhedron* - granular-style 3d polyhedron potential
- *bop* - BOP potential of Pettifor
- *born* - Born-Mayer-Huggins potential
- *born/coul/dsf* - Born with damped-shifted-force model
- *born/coul/dsf/cs* - Born with damped-shifted-force and core/shell model
- *born/coul/long* - Born with long-range Coulombics
- *born/coul/long/cs* - Born with long-range Coulombics and core/shell
- *born/coul/msm* - Born with long-range MSM Coulombics
- *born/coul/wolf* - Born with Wolf potential for Coulombics

- *born/coul/wolf/cs* - Born with Wolf potential for Coulombics and core/shell model
- *brownian* - Brownian potential for Fast Lubrication Dynamics
- *brownian/poly* - Brownian potential for Fast Lubrication Dynamics with polydispersity
- *buck* - Buckingham potential
- *buck/coul/cut* - Buckingham with cutoff Coulomb
- *buck/coul/long* - Buckingham with long-range Coulombics
- *buck/coul/long/cs* - Buckingham with long-range Coulombics and core/shell
- *buck/coul/msm* - Buckingham with long-range MSM Coulombics
- *buck/long/coul/long* - long-range Buckingham with long-range Coulombics
- *buck/mdf* - Buckingham with a taper function
- *buck6d/coul/gauss/dsf* - dispersion-damped Buckingham with damped-shift-force model
- *buck6d/coul/gauss/long* - dispersion-damped Buckingham with long-range Coulombics
- *colloid* - integrated colloidal potential
- *comb* - charge-optimized many-body (COMB) potential
- *comb3* - charge-optimized many-body (COMB3) potential
- *cosine/squared* - Cooke-Kremer-Deserno membrane model potential
- *coul/cut* - cutoff Coulombic potential
- *coul/cut/soft* - Coulombic potential with a soft core
- *coul/debye* - cutoff Coulombic potential with Debye screening
- *coul/diel* - Coulomb potential with dielectric permittivity
- *coul/dsf* - Coulombics with damped-shifted-force model
- *coul/long* - long-range Coulombic potential
- *coul/long/cs* - long-range Coulombic potential and core/shell
- *coul/long/soft* - long-range Coulombic potential with a soft core
- *coul/msm* - long-range MSM Coulombics
- *coul/shield* - Coulombics for boron nitride for use with *ilp/graphene/hbn* potential
- *coul/streitz* - Coulombics via Streitz/Mintmire Slater orbitals
- *coul/wolf* - Coulombics via Wolf potential
- *coul/wolf/cs* - ditto with core/shell adjustments
- *dpd* - dissipative particle dynamics (DPD)
- *dpd/fdt* - DPD for constant temperature and pressure
- *dpd/fdt/energy* - DPD for constant energy and enthalpy
- *dpd/tstat* - pair-wise DPD thermostatting
- *dsmc* - Direct Simulation Monte Carlo (DSMC)
- *e3b* - Explicit-three body (E3B) water model
- *drip* - Dihedral-angle-corrected registry-dependent interlayer potential (DRIP)

- *eam* - embedded atom method (EAM)
- *eam/alloy* - alloy EAM
- *eam/cd* - concentration-dependent EAM
- *eam/cd/old* - older two-site model for concentration-dependent EAM
- *eam/fs* - Finnis-Sinclair EAM
- *edip* - three-body EDIP potential
- *edip/multi* - multi-element EDIP potential
- *edpd* - eDPD particle interactions
- *eff/cut* - electron force field with a cutoff
- *eim* - embedded ion method (EIM)
- *exp6/rx* - reactive DPD potential
- *extep* - extended Tersoff potential
- *gauss* - Gaussian potential
- *gauss/cut* - generalized Gaussian potential
- *gayberne* - Gay-Berne ellipsoidal potential
- *granular* - Generalized granular potential
- *gran/hertz/history* - granular potential with Hertzian interactions
- *gran/hooke* - granular potential with history effects
- *gran/hooke/history* - granular potential without history effects
- *gw* - Gao-Weber potential
- *gw/zbl* - Gao-Weber potential with a repulsive ZBL core
- *hbond/dreiding/lj* - DREIDING hydrogen bonding LJ potential
- *hbond/dreiding/morse* - DREIDING hydrogen bonding Morse potential
- *ilp/graphene/hbn* - registry-dependent interlayer potential (ILP)
- *kim* - interface to potentials provided by KIM project
- *kolmogorov/crespi/full* - Kolmogorov-Crespi (KC) potential with no simplifications
- *kolmogorov/crespi/z* - Kolmogorov-Crespi (KC) potential with normals along z-axis
- *lcbop* - long-range bond-order potential (LCBOP)
- *lebedeva/z* - Lebedeva interlayer potential for graphene with normals along z-axis
- *lennard/mdf* - LJ potential in A/B form with a taper function
- *line/lj* - LJ potential between line segments
- *list* - potential between pairs of atoms explicitly listed in an input file
- *lj/charmm/coul/charmm* - CHARMM potential with cutoff Coulomb
- *lj/charmm/coul/charmm/implicit* - CHARMM for implicit solvent
- *lj/charmm/coul/long* - CHARMM with long-range Coulomb
- *lj/charmm/coul/long/soft* - CHARMM with long-range Coulomb and a soft core

- *lj/charmm/coul/msm* - CHARMM with long-range MSM Coulombics
- *lj/charmmfsw/coul/charmmfsh* - CHARMM with force switching and shifting
- *lj/charmmfsw/coul/long* - CHARMM with force switching and long-rnage Coulombics
- *lj/class2* - COMPASS (class 2) force field with no Coulomb
- *lj/class2/coul/cut* - COMPASS with cutoff Coulomb
- *lj/class2/coul/cut/soft* - COMPASS with cutoff Coulomb with a soft core
- *lj/class2/coul/long* - COMPASS with long-range Coulomb
- *lj/class2/coul/long/soft* - COMPASS with long-range Coulomb with a soft core
- *lj/class2/soft* - COMPASS (class 2) force field with no Coulomb with a soft core
- *lj/cubic* - LJ with cubic after inflection point
- *lj/cut* - cutoff Lennard-Jones potential with no Coulomb
- *lj/cut/coul/cut* - LJ with cutoff Coulomb
- *lj/cut/coul/cut/soft* - LJ with cutoff Coulomb with a soft core
- *lj/cut/coul/debye* - LJ with Debye screening added to Coulomb
- *lj/cut/coul/dsf* - LJ with Coulombics via damped shifted forces
- *lj/cut/coul/long* - LJ with long-range Coulombics
- *lj/cut/coul/long/cs* - ditto with core/shell adjustments
- *lj/cut/coul/long/soft* - LJ with long-range Coulombics with a soft core
- *lj/cut/coul/msm* - LJ with long-range MSM Coulombics
- *lj/cut/coul/wolf* - LJ with Coulombics via Wolf potential
- *lj/cut/dipole/cut* - point dipoles with cutoff
- *lj/cut/dipole/long* - point dipoles with long-range Ewald
- *lj/cut/soft* - LJ with a soft core
- *lj/cut/thole/long* - LJ with Coulombics with thole damping
- *lj/cut/tip4p/cut* - LJ with cutoff Coulomb for TIP4P water
- *lj/cut/tip4p/long* - LJ with long-range Coulomb for TIP4P water
- *lj/cut/tip4p/long/soft* - LJ with cutoff Coulomb for TIP4P water with a soft core
- *lj/expand* - Lennard-Jones for variable size particles
- *lj/expand/coul/long* - Lennard-Jones for variable size particles with long-range Coulombics
- *lj/gromacs* - GROMACS-style Lennard-Jones potential
- *lj/gromacs/coul/gromacs* - GROMACS-style LJ and Coulombic potential
- *lj/long/coul/long* - long-range LJ and long-range Coulombics
- *lj/long/dipole/long* - long-range LJ and long-range point dipoles
- *lj/long/tip4p/long* - long-range LJ and long-range Coulombics for TIP4P water
- *lj/mdf* - LJ potential with a taper function
- *lj/sdk* - LJ for SDK coarse-graining

- *lj/sdk/coul/long* - LJ for SDK coarse-graining with long-range Coulombics
- *lj/sdk/coul/msm* - LJ for SDK coarse-graining with long-range Coulombics via MSM
- *lj/sf/dipole/sf* - LJ with dipole interaction with shifted forces
- *lj/smooth* - smoothed Lennard-Jones potential
- *lj/smooth/linear* - linear smoothed LJ potential
- *lj/switch3/coulgauss/long* - smoothed LJ vdW potential with Gaussian electrostatics
- *lj96/cut* - Lennard-Jones 9/6 potential
- *local/density* - generalized basic local density potential
- *lubricate* - hydrodynamic lubrication forces
- *lubricate/poly* - hydrodynamic lubrication forces with polydispersity
- *lubricateU* - hydrodynamic lubrication forces for Fast Lubrication Dynamics
- *lubricateU/poly* - hydrodynamic lubrication forces for Fast Lubrication with polydispersity
- *mdpd* - mDPD particle interactions
- *mdpd/rhosum* - mDPD particle interactions for mass density
- *meam/c* - modified embedded atom method (MEAM) in C
- *meam/spline* - splined version of MEAM
- *meam/sw/spline* - splined version of MEAM with a Stillinger-Weber term
- *mesocnt* - mesoscale model for (carbon) nanotubes
- *mgpt* - simplified model generalized pseudopotential theory (MGPT) potential
- *mie/cut* - Mie potential
- *mm3/switch3/coulgauss/long* - smoothed MM3 vdW potential with Gaussian electrostatics
- *momb* - Many-Body Metal-Organic (MOMB) force field
- *morse* - Morse potential
- *morse/smooth/linear* - linear smoothed Morse potential
- *morse/soft* - Morse potential with a soft core
- *multi/lucy* - DPD potential with density-dependent force
- *multi/lucy/rx* - reactive DPD potential with density-dependent force
- *nb3b/harmonic* - non-bonded 3-body harmonic potential
- *nm/cut* - N-M potential
- *nm/cut/coul/cut* - N-M potential with cutoff Coulomb
- *nm/cut/coul/long* - N-M potential with long-range Coulombics
- *oxdna/coaxstk* -
- *oxdna/excv* -
- *oxdna/hbond* -
- *oxdna/stk* -
- *oxdna/xstk* -

- *oxdna2/coaxstk* -
- *oxdna2/dh* -
- *oxdna2/excv* -
- *oxdna2/hbond* -
- *oxdna2/stk* -
- *oxdna2/xstk* -
- *oxrna2/coaxstk* -
- *oxrna2/dh* -
- *oxrna2/excv* -
- *oxrna2/hbond* -
- *oxrna2/stk* -
- *oxrna2/xstk* -
- *peri/eps* - peridynamic EPS potential
- *peri/lps* - peridynamic LPS potential
- *peri/pmb* - peridynamic PMB potential
- *peri/ves* - peridynamic VES potential
- *polymorphic* - polymorphic 3-body potential
- *python* -
- *quip* -
- *reax/c* - ReaxFF potential in C
- *rebo* - 2nd generation REBO potential of Brenner
- *resquared* - Everaers RE-Squared ellipsoidal potential
- *sdpd/taitwater/isothermal* - smoothed dissipative particle dynamics for water at isothermal conditions
- *smd/hertz* -
- *smd/tlsph* -
- *smd/tri_surface* -
- *smd/ulsph* -
- *smtbq* -
- *snap* - SNAP quantum-accurate potential
- *soft* - Soft (cosine) potential
- *sph/heatconduction* -
- *sph/idealgas* -
- *sph/lj* -
- *sph/rhosum* -
- *sph/taitwater* -
- *sph/taitwater/morris* -

- *spin/dipole/cut* -
- *spin/dipole/long* -
- *spin/dmi* -
- *spin/exchange* -
- *spin/magelec* -
- *spin/neel* -
- *srp* -
- *sw* - Stillinger-Weber 3-body potential
- *table* - tabulated pair potential
- *table/rx* -
- *tdpd* - tDPD particle interactions
- *tersoff* - Tersoff 3-body potential
- *tersoff/mod* - modified Tersoff 3-body potential
- *tersoff/mod/c* -
- *tersoff/table* -
- *tersoff/zbl* - Tersoff/ZBL 3-body potential
- *thole* - Coulomb interactions with thole damping
- *tip4p/cut* - Coulomb for TIP4P water w/out LJ
- *tip4p/long* - long-range Coulombics for TIP4P water w/out LJ
- *tip4p/long/soft* -
- *tri/lj* - LJ potential between triangles
- *ufm* -
- *vashishta* - Vashishta 2-body and 3-body potential
- *vashishta/table* -
- *yukawa* - Yukawa potential
- *yukawa/colloid* - screened Yukawa potential for finite-size particles
- *zbl* - Ziegler-Biersack-Littmark potential

15.89.4 Restrictions

This command must be used before any coefficients are set by the *pair_coeff*, *read_data*, or *read_restart* commands.

Some pair styles are part of specific packages. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info. The doc pages for individual pair potentials tell if it is part of a package.

15.89.5 Related commands

pair_coeff, *read_data*, *pair_modify*, *kspace_style*, *dielectric*, *pair_write*

15.89.6 Default

```
pair_style none
```

15.90 pair_write command

15.90.1 Syntax

```
pair_write itype jtype N style inner outer file keyword Qi Qj
```

- itype,jtype = 2 atom types
- N = # of values
- style = *r* or *rsq* or *bitmap*
- inner,outer = inner and outer cutoff (distance units)
- file = name of file to write values to
- keyword = section name in file for this set of tabulated values
- Qi,Qj = 2 atom charges (charge units) (optional)

15.90.2 Examples

```
pair_write 1 3 500 r 1.0 10.0 table.txt LJ
pair_write 1 1 1000 rsq 2.0 8.0 table.txt Yukawa_1_1 -0.5 0.5
```

15.90.3 Description

Write energy and force values to a file as a function of distance for the currently defined pair potential. This is useful for plotting the potential function or otherwise debugging its values. If the file already exists, the table of values is appended to the end of the file to allow multiple tables of energy and force to be included in one file.

The energy and force values are computed at distances from inner to outer for 2 interacting atoms of type itype and jtype, using the appropriate *pair_coeff* coefficients. If the style is *r*, then N distances are used, evenly spaced in r; if the style is *rsq*, N distances are used, evenly spaced in r^2.

For example, for N = 7, style = *r*, inner = 1.0, and outer = 4.0, values are computed at r = 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0.

If the style is *bitmap*, then 2^N values are written to the file in a format and order consistent with how they are read in by the *pair_coeff* command for pair style *table*. For reasonable accuracy in a bitmapped table, choose N >= 12, an *inner* value that is smaller than the distance of closest approach of 2 atoms, and an *outer* value <= cutoff of the potential.

If the pair potential is computed between charged atoms, the charges of the pair of interacting atoms can optionally be specified. If not specified, values of Qi = Qj = 1.0 are used.

The file is written in the format used as input for the *pair_style table* option with *keyword* as the section name. Each line written to the file lists an index number (1-N), a distance (in distance units), an energy (in energy units), and a force (in force units).

15.90.4 Restrictions

All force field coefficients for pair and other kinds of interactions must be set before this command can be invoked.

Due to how the pairwise force is computed, an inner value > 0.0 must be specified even if the potential has a finite value at r = 0.0.

For EAM potentials, the pair_write command only tabulates the pairwise portion of the potential, not the embedding portion.

15.90.5 Related commands

pair_style table, *pair_style*, *pair_coeff*

Default: none

15.91 partition command

15.91.1 Syntax

```
partition style N command ...
```

- style = *yes* or *no*
- N = partition number (see asterisk form below)
- command = any LAMMPS command

15.91.2 Examples

```
partition yes 1 processors 4 10 6
partition no 5 print "Active partition"
partition yes *5 fix all nve
partition yes 6* fix all nvt temp 1.0 1.0 0.1
```

15.91.3 Description

This command invokes the specified command on a subset of the partitions of processors you have defined via the *-partition command-line switch*.

Normally, every input script command in your script is invoked by every partition. This behavior can be modified by defining world- or universe-style *variables* that have different values for each partition. This mechanism can be used to cause your script to jump to different input script files on different partitions, if such a variable is used in a *jump* command.

The "partition" command is another mechanism for having as input script operate differently on different partitions. It is basically a prefix on any LAMMPS command. The command will only be invoked on the partition(s) specified by the *style* and *N* arguments.

If the *style* is *yes*, the command will be invoked on any partition which matches the *N* argument. If the *style* is *no* the command will be invoked on all the partitions which do not match the Np argument.

Partitions are numbered from 1 to Np, where Np is the number of partitions specified by the *-partition command-line switch*.

N can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to span a range of partition numbers. This takes the form "*" or "*n" or "n*" or "m*n". An asterisk with no numeric values means all partitions from 1 to Np. A leading asterisk means all partitions from 1 to n (inclusive). A trailing asterisk means all partitions from n to Np (inclusive). A middle asterisk means all partitions from m to n (inclusive).

This command can be useful for the "run_style verlet/split" command which imposed requirements on how the *processors* command lays out a 3d grid of processors in each of 2 partitions.

15.91.4 Restrictions

none

15.91.5 Related commands

run_style verlet/split

Default: none

15.92 prd command

15.92.1 Syntax

```
prd N t_event n_dephase t_dephase t_correlate compute-ID seed keyword value ...
```

- N = # of timesteps to run (not including dephasing/quenching)
- t_event = timestep interval between event checks
- n_dephase = number of velocity randomizations to perform in each dephase run
- t_dephase = number of timesteps to run dynamics after each velocity randomization during dephase
- t_correlate = number of timesteps within which 2 consecutive events are considered to be correlated
- compute-ID = ID of the compute used for event detection
- random_seed = random # seed (positive integer)
- zero or more keyword/value pairs may be appended
- keyword = *min* or *temp* or *vel*

```
min values = etol ftol maxiter maxeval
  etol = stopping tolerance for energy, used in quenching
  ftol = stopping tolerance for force, used in quenching
  maxiter = max iterations of minimize, used in quenching
  maxeval = max number of force/energy evaluations, used in quenching
temp value = Tdephase
  Tdephase = target temperature for velocity randomization, used in␣
↪dephasing
```

```
    vel values = loop dist
      loop = all or local or geom, used in dephasing
      dist = uniform or gaussian, used in dephasing
    time value = steps or clock
      steps = simulation runs for N timesteps on each replica (default)
      clock = simulation runs for N timesteps across all replicas
```

15.92.2 Examples

```
prd 5000 100 10 10 100 1 54982
prd 5000 100 10 10 100 1 54982 min 0.1 0.1 100 200
```

15.92.3 Description

Run a parallel replica dynamics (PRD) simulation using multiple replicas of a system. One or more replicas can be used. The total number of steps *N* to run can be interpreted in one of two ways; see discussion of the *time* keyword below.

PRD is described in *(Voter1998)* by Art Voter. Similar to global or local hyperdynamics (HD), PRD is a method for performing accelerated dynamics that is suitable for infrequent-event systems that obey first-order kinetics. A good overview of accelerated dynamics methods for such systems in given in this review paper *(Voter2002)* from Art's group. To quote from the paper: "The dynamical evolution is characterized by vibrational excursions within a potential basin, punctuated by occasional transitions between basins." The transition probability is characterized by p(t) = k*exp(-kt) where k is the rate constant. Running multiple replicas gives an effective enhancement in the timescale spanned by the multiple simulations, while waiting for an event to occur.

Both PRD and HD produce a time-accurate trajectory that effectively extends the timescale over which a system can be simulated, but they do it differently. PRD creates Nr replicas of the system and runs dynamics on each independently with a normal unbiased potential until an event occurs in one of the replicas. The time between events is reduced by a factor of Nr replicas. HD uses a single replica of the system and accelerates time by biasing the interaction potential in a manner such that each timestep is effectively longer. For both methods, per CPU second, more physical time elapses and more events occur. See the *hyper* doc page for more info about HD.

In PRD, each replica runs on a partition of one or more processors. Processor partitions are defined at run-time using the *-partition command-line switch*. Note that if you have MPI installed, you can run a multi-replica simulation with more replicas (partitions) than you have physical processors, e.g you can run a 10-replica simulation on one or two processors. However for PRD, this makes little sense, since running a replica on virtual instead of physical processors,offers no effective parallel speed-up in searching for infrequent events. See the *Howto replica* doc page for further discussion.

When a PRD simulation is performed, it is assumed that each replica is running the same model, though LAMMPS does not check for this. I.e. the simulation domain, the number of atoms, the interaction potentials, etc should be the same for every replica.

A PRD run has several stages, which are repeated each time an "event" occurs in one of the replicas, as explained below. The logic for a PRD run is as follows:

```
while (time remains):
  dephase for n_dephase*t_dephase steps
  until (event occurs on some replica):
    run dynamics for t_event steps
    quench
    check for uncorrelated event on any replica
  until (no correlated event occurs):
    run dynamics for t_correlate steps
```

```
    quench
    check for correlated event on this replica
  event replica shares state with all replicas
```

Before this loop begins, the state of the system on replica 0 is shared with all replicas, so that all replicas begin from the same initial state. The first potential energy basin is identified by quenching (an energy minimization, see below) the initial state and storing the resulting coordinates for reference.

In the first stage, dephasing is performed by each replica independently to eliminate correlations between replicas. This is done by choosing a random set of velocities, based on the *random_seed* that is specified, and running *t_dephase* timesteps of dynamics. This is repeated *n_dephase* times. At each of the *n_dephase* stages, if an event occurs during the *t_dephase* steps of dynamics for a particular replica, the replica repeats the stage until no event occurs.

If the *temp* keyword is not specified, the target temperature for velocity randomization for each replica is the current temperature of that replica. Otherwise, it is the specified *Tdephase* temperature. The style of velocity randomization is controlled using the keyword *vel* with arguments that have the same meaning as their counterparts in the *velocity* command.

In the second stage, each replica runs dynamics continuously, stopping every *t_event* steps to check if a transition event has occurred. This check is performed by quenching the system and comparing the resulting atom coordinates to the coordinates from the previous basin. The first time through the PRD loop, the "previous basin" is the set of quenched coordinates from the initial state of the system.

A quench is an energy minimization and is performed by whichever algorithm has been defined by the *min_style* command. Minimization parameters may be set via the *min_modify* command and by the *min* keyword of the PRD command. The latter are the settings that would be used with the *minimize* command. Note that typically, you do not need to perform a highly-converged minimization to detect a transition event, though you may need to in order to prevent a set of atoms in the system from relaxing to a saddle point.

The event check is performed by a compute with the specified *compute-ID*. Currently there is only one compute that works with the PRD command, which is the *compute event/displace* command. Other event-checking computes may be added. *Compute event/displace* checks whether any atom in the compute group has moved further than a specified threshold distance. If so, an "event" has occurred.

In the third stage, the replica on which the event occurred (event replica) continues to run dynamics to search for correlated events. This is done by running dynamics for *t_correlate* steps, quenching every *t_event* steps, and checking if another event has occurred.

The first time no correlated event occurs, the final state of the event replica is shared with all replicas, the new basin reference coordinates are updated with the quenched state, and the outer loop begins again. While the replica event is searching for correlated events, all the other replicas also run dynamics and event checking with the same schedule, but the final states are always overwritten by the state of the event replica.

The outer loop of the pseudo-code above continues until *N* steps of dynamics have been performed. Note that *N* only includes the dynamics of stages 2 and 3, not the steps taken during dephasing or the minimization iterations of quenching. The specified *N* is interpreted in one of two ways, depending on the *time* keyword. If the *time* value is *steps*, which is the default, then each replica runs for *N* timesteps. If the *time* value is *clock*, then the simulation runs until *N* aggregate timesteps across all replicas have elapsed. This aggregate time is the "clock" time defined below, which typically advances nearly M times faster than the timestepping on a single replica, where M is the number of replicas.

Four kinds of output can be generated during a PRD run: event statistics, thermodynamic output by each replica, dump files, and restart files.

When running with multiple partitions (each of which is a replica in this case), the print-out to the screen and master log.lammps file is limited to event statistics. Note that if a PRD run is performed on only a single replica then the event statistics will be intermixed with the usual thermodynamic output discussed below.

The quantities printed each time an event occurs are the timestep, CPU time, clock, event number, a correlation flag, the number of coincident events, and the replica number of the chosen event.

The timestep is the usual LAMMPS timestep, except that time does not advance during dephasing or quenches, but only during dynamics. Note that are two kinds of dynamics in the PRD loop listed above that contribute to this timestepping. The first is when all replicas are performing independent dynamics, waiting for an event to occur. The second is when correlated events are being searched for, but only one replica is running dynamics.

The CPU time is the total elapsed time on each processor, since the start of the PRD run.

The clock is the same as the timestep except that it advances by M steps per timestep during the first kind of dynamics when the M replicas are running independently. The clock advances by only 1 step per timestep during the second kind of dynamics, when only a single replica is checking for a correlated event. Thus "clock" time represents the aggregate time (in steps) that has effectively elapsed during a PRD simulation on M replicas. If most of the PRD run is spent in the second stage of the loop above, searching for infrequent events, then the clock will advance nearly M times faster than it would if a single replica was running. Note the clock time between successive events should be drawn from p(t).

The event number is a counter that increments with each event, whether it is uncorrelated or correlated.

The correlation flag will be 0 when an uncorrelated event occurs during the second stage of the loop listed above, i.e. when all replicas are running independently. The correlation flag will be 1 when a correlated event occurs during the third stage of the loop listed above, i.e. when only one replica is running dynamics.

When more than one replica detects an event at the end of the same event check (every *t_event* steps) during the second stage, then one of them is chosen at random. The number of coincident events is the number of replicas that detected an event. Normally, this value should be 1. If it is often greater than 1, then either the number of replicas is too large, or *t_event* is too large.

The replica number is the ID of the replica (from 0 to M-1) in which the event occurred.

When running on multiple partitions, LAMMPS produces additional log files for each partition, e.g. log.lammps.0, log.lammps.1, etc. For the PRD command, these contain the thermodynamic output for each replica. You will see short runs and minimizations corresponding to the dynamics and quench operations of the loop listed above. The timestep will be reset appropriately depending on whether the operation advances time or not.

After the PRD command completes, timing statistics for the PRD run are printed in each replica's log file, giving a breakdown of how much CPU time was spent in each stage (dephasing, dynamics, quenching, etc).

Any *dump files* defined in the input script, will be written to during a PRD run at timesteps corresponding to both uncorrelated and correlated events. This means the requested dump frequency in the *dump* command is ignored. There will be one dump file (per dump command) created for all partitions.

The atom coordinates of the dump snapshot are those of the minimum energy configuration resulting from quenching following a transition event. The timesteps written into the dump files correspond to the timestep at which the event occurred and NOT the clock. A dump snapshot corresponding to the initial minimum state used for event detection is written to the dump file at the beginning of each PRD run.

If the *restart* command is used, a single restart file for all the partitions is generated, which allows a PRD run to be continued by a new input script in the usual manner.

The restart file is generated at the end of the loop listed above. If no correlated events are found, this means it contains a snapshot of the system at time T + *t_correlate*, where T is the time at which the uncorrelated event occurred. If correlated events were found, then it contains a snapshot of the system at time T + *t_correlate*, where T is the time of the last correlated event.

The restart frequency specified in the *restart* command is interpreted differently when performing a PRD run. It does not mean the timestep interval between restart files. Instead it means an event interval for uncorrelated events. Thus a frequency of 1 means write a restart file every time an uncorrelated event occurs. A frequency of 10 means write a restart file every 10th uncorrelated event.

When an input script reads a restart file from a previous PRD run, the new script can be run on a different number of replicas or processors. However, it is assumed that *t_correlate* in the new PRD command is the same as it was previously. If not, the calculation of the "clock" value for the first event in the new run will be slightly off.

15.92.4 Restrictions

This command can only be used if LAMMPS was built with the REPLICA package. See the *Build package* doc page for more info.

The *N* and *t_correlate* settings must be integer multiples of *t_event*.

Runs restarted from restart file written during a PRD run will not produce identical results due to changes in the random numbers used for dephasing.

This command cannot be used when any fixes are defined that keep track of elapsed time to perform time-dependent operations. Examples include the "ave" fixes such as *fix ave/chunk*. Also *fix dt/reset* and *fix deposit*.

15.92.5 Related commands

compute event/displace, *min_modify*, *min_style*, *run_style*, *minimize*, *velocity*, *temper*, *neb*, *tad*, *hyper*

15.92.6 Default

The option defaults are min = 0.1 0.1 40 50, no temp setting, vel = geom gaussian, and time = steps.

(Voter1998) Voter, Phys Rev B, 57, 13985 (1998).

(Voter2002) Voter, Montalenti, Germann, Annual Review of Materials Research 32, 321 (2002).

15.93 print command

15.93.1 Syntax

```
print string keyword value
```

- string = text string to print, which may contain variables
- zero or more keyword/value pairs may be appended
- keyword = *file* or *append* or *screen* or *universe*

  ```
  file value = filename
  append value = filename
  screen value = yes or no
  universe value = yes or no
  ```

15.93.2 Examples

```
print "Done with equilibration" file info.dat
print Vol=$v append info.dat screen no
print "The system volume is now $v"
print 'The system volume is now $v'
print "NEB calculation 1 complete" screen no universe yes
print """
System volume = $v
System temperature = $t
"""
```

15.93.3 Description

Print a text string to the screen and logfile. The text string must be a single argument, so if it is one line but more than one word, it should be enclosed in single or double quotes. To generate multiple lines of output, the string can be enclosed in triple quotes, as in the last example above. If the text string contains variables, they will be evaluated and their current values printed.

If the *file* or *append* keyword is used, a filename is specified to which the output will be written. If *file* is used, then the filename is overwritten if it already exists. If *append* is used, then the filename is appended to if it already exists, or created if it does not exist.

If the *screen* keyword is used, output to the screen and logfile can be turned on or off as desired.

If the *universe* keyword is used, output to the global screen and logfile can be turned on or off as desired. In multi-partition calculations, the *screen* option and the corresponding output only apply to the screen and logfile of the individual partition.

If you want the print command to be executed multiple times (with changing variable values), there are 3 options. First, consider using the *fix print* command, which will print a string periodically during a simulation. Second, the print command can be used as an argument to the *every* option of the *run* command. Third, the print command could appear in a section of the input script that is looped over (see the *jump* and *next* commands).

See the *variable* command for a description of *equal* style variables which are typically the most useful ones to use with the print command. Equal-style variables can calculate formulas involving mathematical operations, atom properties, group properties, thermodynamic properties, global values calculated by a *compute* or *fix*, or references to other *variables*.

15.93.4 Restrictions

none

15.93.5 Related commands

fix print, *variable*

15.93.6 Default

The option defaults are no file output, screen = yes, and universe = no.

15.94 processors command

15.94.1 Syntax

```
processors Px Py Pz keyword args ...
```

- Px,Py,Pz = # of processors in each dimension of 3d grid overlaying the simulation domain
- zero or more keyword/arg pairs may be appended
- keyword = *grid* or *map* or *part* or *file*

```
grid arg = gstyle params ...
  gstyle = onelevel or twolevel or numa or custom
    onelevel params = none
    twolevel params = Nc Cx Cy Cz
      Nc = number of cores per node
      Cx,Cy,Cz = # of cores in each dimension of 3d sub-grid assigned to␣
↪each node
    numa params = none
    custom params = infile
      infile = file containing grid layout
map arg = cart or cart/reorder or xyz or xzy or yxz or yzx or zxy or zyx
   cart = use MPI_Cart() methods to map processors to 3d grid with␣
↪reorder = 0
   cart/reorder = use MPI_Cart() methods to map processors to 3d grid␣
↪with reorder = 1
   xyz,xzy,yxz,yzx,zxy,zyx = map processors to 3d grid in IJK ordering
numa arg = none
part args = Psend Precv cstyle
  Psend = partition # (1 to Np) which will send its processor layout
  Precv = partition # (1 to Np) which will recv the processor layout
  cstyle = multiple
    multiple = Psend grid will be multiple of Precv grid in each dimension
file arg = outfile
  outfile = name of file to write 3d grid of processors to
```

15.94.2 Examples

```
processors * * 5
processors 2 4 4
processors * * 8 map xyz
processors * * * grid numa
processors * * * grid twolevel 4 * * 1
processors 4 8 16 grid custom myfile
processors * * * part 1 2 multiple
```

15.94.3 Description

Specify how processors are mapped as a regular 3d grid to the global simulation box. The mapping involves 2 steps. First if there are P processors it means choosing a factorization P = Px by Py by Pz so that there are Px processors in the x dimension, and similarly for the y and z dimensions. Second, the P processors are mapped to the regular 3d grid. The arguments to this command control each of these 2 steps.

The Px, Py, Pz parameters affect the factorization. Any of the 3 parameters can be specified with an asterisk "*", which means LAMMPS will choose the number of processors in that dimension of the grid. It will do this based on the size and shape of the global simulation box so as to minimize the surface-to-volume ratio of each processor's sub-domain.

Choosing explicit values for Px or Py or Pz can be used to override the default manner in which LAMMPS will create the regular 3d grid of processors, if it is known to be sub-optimal for a particular problem. E.g. a problem where the extent of atoms will change dramatically in a particular dimension over the course of the simulation.

The product of Px, Py, Pz must equal P, the total # of processors LAMMPS is running on. For a *2d simulation*, Pz must equal 1.

Note that if you run on a prime number of processors P, then a grid such as 1 x P x 1 will be required, which may incur extra communication costs due to the high surface area of each processor's sub-domain.

Also note that if multiple partitions are being used then P is the number of processors in this partition; see the *-partition command-line switch* doc page for details. Also note that you can prefix the processors command with the *partition* command to easily specify different Px,Py,Pz values for different partitions.

You can use the *partition* command to specify different processor grids for different partitions, e.g.

```
partition yes 1 processors 4 4 4
partition yes 2 processors 2 3 2
```

Note: This command only affects the initial regular 3d grid created when the simulation box is first specified via a *create_box* or *read_data* or *read_restart* command. Or if the simulation box is re-created via the *replicate* command. The same regular grid is initially created, regardless of which *comm_style* command is in effect.

If load-balancing is never invoked via the *balance* or *fix balance* commands, then the initial regular grid will persist for all simulations. If balancing is performed, some of the methods invoked by those commands retain the logical topology of the initial 3d grid, and the mapping of processors to the grid specified by the processors command. However the grid spacings in different dimensions may change, so that processors own sub-domains of different sizes. If the *comm_style tiled* command is used, methods invoked by the balancing commands may discard the 3d grid of processors and tile the simulation domain with sub-domains of different sizes and shapes which no longer have a logical 3d connectivity. If that occurs, all the information specified by the processors command is ignored.

The *grid* keyword affects the factorization of P into Px,Py,Pz and it can also affect how the P processor IDs are mapped to the 3d grid of processors.

The *onelevel* style creates a 3d grid that is compatible with the Px,Py,Pz settings, and which minimizes the surface-to-volume ratio of each processor's sub-domain, as described above. The mapping of processors to the grid is determined by the *map* keyword setting.

The *twolevel* style can be used on machines with multicore nodes to minimize off-node communication. It insures that contiguous sub-sections of the 3d grid are assigned to all the cores of a node. For example if *Nc* is 4, then 2x2x1 or 2x1x2 or 1x2x2 sub-sections of the 3d grid will correspond to the cores of each node. This affects both the factorization and mapping steps.

The *Cx*, *Cy*, *Cz* settings are similar to the *Px*, *Py*, *Pz* settings, only their product should equal *Nc*. Any of the 3 parameters can be specified with an asterisk "*", which means LAMMPS will choose the number of cores in that

dimension of the node's sub-grid. As with Px,Py,Pz, it will do this based on the size and shape of the global simulation box so as to minimize the surface-to-volume ratio of each processor's sub-domain.

Note: For the *twolevel* style to work correctly, it assumes the MPI ranks of processors LAMMPS is running on are ordered by core and then by node. E.g. if you are running on 2 quad-core nodes, for a total of 8 processors, then it assumes processors 0,1,2,3 are on node 1, and processors 4,5,6,7 are on node 2. This is the default rank ordering for most MPI implementations, but some MPIs provide options for this ordering, e.g. via environment variable settings.

The *numa* style operates similar to the *twolevel* keyword except that it auto-detects which cores are running on which nodes. Currently, it does this in only 2 levels, but it may be extended in the future to account for socket topology and other non-uniform memory access (NUMA) costs. It also uses a different algorithm than the *twolevel* keyword for doing the two-level factorization of the simulation box into a 3d processor grid to minimize off-node communication, and it does its own MPI-based mapping of nodes and cores to the regular 3d grid. Thus it may produce a different layout of the processors than the *twolevel* options.

The *numa* style will give an error if the number of MPI processes is not divisible by the number of cores used per node, or any of the Px or Py of Pz values is greater than 1.

Note: Unlike the *twolevel* style, the *numa* style does not require any particular ordering of MPI ranks i norder to work correctly. This is because it auto-detects which processes are running on which nodes.

The *custom* style uses the file *infile* to define both the 3d factorization and the mapping of processors to the grid.

The file should have the following format. Any number of initial blank or comment lines (starting with a "#" character) can be present. The first non-blank, non-comment line should have 3 values:

```
Px Py Py
```

These must be compatible with the total number of processors and the Px, Py, Pz settings of the processors command.

This line should be immediately followed by P = Px*Py*Pz lines of the form:

```
ID I J K
```

where ID is a processor ID (from 0 to P-1) and I,J,K are the processors location in the 3d grid. I must be a number from 1 to Px (inclusive) and similarly for J and K. The P lines can be listed in any order, but no processor ID should appear more than once.

The *map* keyword affects how the P processor IDs (from 0 to P-1) are mapped to the 3d grid of processors. It is only used by the *onelevel* and *twolevel* grid settings.

The *cart* style uses the family of MPI Cartesian functions to perform the mapping, namely MPI_Cart_create(), MPI_Cart_get(), MPI_Cart_shift(), and MPI_Cart_rank(). It invokes the MPI_Cart_create() function with its reorder flag = 0, so that MPI is not free to reorder the processors.

The *cart/reorder* style does the same thing as the *cart* style except it sets the reorder flag to 1, so that MPI can reorder processors if it desires.

The *xyz*, *xzy*, *yxz*, *yzx*, *zxy*, and *zyx* styles are all similar. If the style is IJK, then it maps the P processors to the grid so that the processor ID in the I direction varies fastest, the processor ID in the J direction varies next fastest, and the processor ID in the K direction varies slowest. For example, if you select style *xyz* and you have a 2x2x2 grid of 8 processors, the assignments of the 8 octants of the simulation domain will be:

```
proc 0 = lo x, lo y, lo z octant
proc 1 = hi x, lo y, lo z octant
proc 2 = lo x, hi y, lo z octant
proc 3 = hi x, hi y, lo z octant
proc 4 = lo x, lo y, hi z octant
proc 5 = hi x, lo y, hi z octant
proc 6 = lo x, hi y, hi z octant
proc 7 = hi x, hi y, hi z octant
```

Note that, in principle, an MPI implementation on a particular machine should be aware of both the machine's network topology and the specific subset of processors and nodes that were assigned to your simulation. Thus its MPI_Cart calls can optimize the assignment of MPI processes to the 3d grid to minimize communication costs. In practice, however, few if any MPI implementations actually do this. So it is likely that the *cart* and *cart/reorder* styles simply give the same result as one of the IJK styles.

Also note, that for the *twolevel* grid style, the *map* setting is used to first map the nodes to the 3d grid, then again to the cores within each node. For the latter step, the *cart* and *cart/reorder* styles are not supported, so an *xyz* style is used in their place.

The *part* keyword affects the factorization of P into Px,Py,Pz.

It can be useful when running in multi-partition mode, e.g. with the *run_style verlet/split* command. It specifies a dependency between a sending partition *Psend* and a receiving partition *Precv* which is enforced when each is setting up their own mapping of their processors to the simulation box. Each of *Psend* and *Precv* must be integers from 1 to Np, where Np is the number of partitions you have defined via the *-partition command-line switch*.

A "dependency" means that the sending partition will create its regular 3d grid as Px by Py by Pz and after it has done this, it will send the Px,Py,Pz values to the receiving partition. The receiving partition will wait to receive these values before creating its own regular 3d grid and will use the sender's Px,Py,Pz values as a constraint. The nature of the constraint is determined by the *cstyle* argument.

For a *cstyle* of *multiple*, each dimension of the sender's processor grid is required to be an integer multiple of the corresponding dimension in the receiver's processor grid. This is a requirement of the *run_style verlet/split* command.

For example, assume the sending partition creates a 4x6x10 grid = 240 processor grid. If the receiving partition is running on 80 processors, it could create a 4x2x10 grid, but it will not create a 2x4x10 grid, since in the y-dimension, 6 is not an integer multiple of 4.

Note: If you use the *partition* command to invoke different "processors" commands on different partitions, and you also use the *part* keyword, then you must insure that both the sending and receiving partitions invoke the "processors" command that connects the 2 partitions via the *part* keyword. LAMMPS cannot easily check for this, but your simulation will likely hang in its setup phase if this error has been made.

The *file* keyword writes the mapping of the factorization of P processors and their mapping to the 3d grid to the specified file *outfile*. This is useful to check that you assigned physical processors in the manner you desired, which can be tricky to figure out, especially when running on multiple partitions or on, a multicore machine or when the processor ranks were reordered by use of the *-reorder command-line switch* or due to use of MPI-specific launch options such as a config file.

If you have multiple partitions you should insure that each one writes to a different file, e.g. using a *world-style variable* for the filename. The file has a self-explanatory header, followed by one-line per processor in this format:

world-ID universe-ID original-ID: I J K: name

The IDs are the processor's rank in this simulation (the world), the universe (of multiple simulations), and the original MPI communicator used to instantiate LAMMPS, respectively. The world and universe IDs will only be different if you are running on more than one partition; see the *-partition command-line switch*. The universe and original IDs will only be different if you used the *-reorder command-line switch* to reorder the processors differently than their rank in the original communicator LAMMPS was instantiated with.

I,J,K are the indices of the processor in the regular 3d grid, each from 1 to Nd, where Nd is the number of processors in that dimension of the grid.

The *name* is what is returned by a call to MPI_Get_processor_name() and should represent an identifier relevant to the physical processors in your machine. Note that depending on the MPI implementation, multiple cores can have the same *name*.

15.94.4 Restrictions

This command cannot be used after the simulation box is defined by a *read_data* or *create_box* command. It can be used before a restart file is read to change the 3d processor grid from what is specified in the restart file.

The *grid numa* keyword only currently works with the *map cart* option.

The *part* keyword (for the receiving partition) only works with the *grid onelevel* or *grid twolevel* options.

15.94.5 Related commands

partition, *-reorder command-line switch*

15.94.6 Default

The option defaults are Px Py Pz = * * *, grid = onelevel, and map = cart.

15.95 python command

15.95.1 Syntax

```
python func keyword args ...
```

- func = name of Python function
- one or more keyword/args pairs must be appended

```
keyword = invoke or input or return or format or length or file or here␣
↪or exists or source
  invoke arg = none = invoke the previously defined Python function
  input args = N i1 i2 ... iN
    N = # of inputs to function
    i1,...,iN = value, SELF, or LAMMPS variable name
      value = integer number, floating point number, or string
      SELF = reference to LAMMPS itself which can be accessed by Python␣
↪function
      variable = v_name, where name = name of LAMMPS variable, e.g. v_abc
  return arg = varReturn
```

```
      varReturn = v_name  = LAMMPS variable name which return value of␣
↪function will be assigned to
    format arg = fstring with M characters
      M = N if no return value, where N = # of inputs
      M = N+1 if there is a return value
      fstring = each character (i,f,s,p) corresponds in order to an input␣
↪or return value
      'i' = integer, 'f' = floating point, 's' = string, 'p' = SELF
    length arg = Nlen
      Nlen = max length of string returned from Python function
    file arg = filename
      filename = file of Python code, which defines func
    here arg = inline
      inline = one or more lines of Python code which defines func
               must be a single argument, typically enclosed between triple␣
↪quotes
    exists arg = none = Python code has been loaded by previous python␣
↪command
    source arg = filename or inline
      filename = file of Python code which will be executed immediately
      inline = one or more lines of Python code which will be executed␣
↪immediately
               must be a single argument, typically enclosed between triple␣
↪quotes
```

15.95.2 Examples

```
python pForce input 2 v_x 20.0 return v_f format fff file force.py
python pForce invoke

python factorial input 1 myN return v_fac format ii here """
def factorial(n):
  if n == 1: return n
  return n * factorial(n-1)
 """

python loop input 1 SELF return v_value format pf here """
def loop(lmpptr,N,cut0):
  from lammps import lammps
  lmp = lammps(ptr=lmpptr)

  # loop N times, increasing cutoff each time

  for i in range(N):
    cut = cut0 + i*0.1
    lmp.set_variable("cut",cut)                # set a variable in LAMMPS
    lmp.command("pair_style lj/cut ${cut}")    # LAMMPS commands
    lmp.command("pair_coeff * * 1.0 1.0")
    lmp.command("run 100")
 """
```

15.95.3 Description

Define a Python function or execute a previously defined function or execute some arbitrary python code. Arguments, including LAMMPS variables, can be passed to the function from the LAMMPS input script and a value returned by the Python function to a LAMMPS variable. The Python code for the function can be included directly in the input script or in a separate Python file. The function can be standard Python code or it can make "callbacks" to LAMMPS through its library interface to query or set internal values within LAMMPS. This is a powerful mechanism for performing complex operations in a LAMMPS input script that are not possible with the simple input script and variable syntax which LAMMPS defines. Thus your input script can operate more like a true programming language.

Use of this command requires building LAMMPS with the PYTHON package which links to the Python library so that the Python interpreter is embedded in LAMMPS. More details about this process are given below.

There are two ways to invoke a Python function once it has been defined. One is using the *invoke* keyword. The other is to assign the function to a *python-style variable* defined in your input script. Whenever the variable is evaluated, it will execute the Python function to assign a value to the variable. Note that variables can be evaluated in many different ways within LAMMPS. They can be substituted for directly in an input script. Or they can be passed to various commands as arguments, so that the variable is evaluated during a simulation run.

A broader overview of how Python can be used with LAMMPS is given on the *Python* doc page. There is an examples/python directory which illustrates use of the python command.

The *func* setting specifies the name of the Python function. The code for the function is defined using the *file* or *here* keywords as explained below. In case of the *source* keyword, the name of the function is ignored.

If the *invoke* keyword is used, no other keywords can be used, and a previous python command must have defined the Python function referenced by this command. This invokes the Python function with the previously defined arguments and return value processed as explained below. You can invoke the function as many times as you wish in your input script.

If the *source* keyword is used, no other keywords can be used. The argument can be a filename or a string with python commands, either on a single line enclosed in quotes, or as multiple lines enclosed in triple quotes. These python commands will be passed to the python interpreter and executed immediately without registering a python function for future execution.

The *input* keyword defines how many arguments *N* the Python function expects. If it takes no arguments, then the *input* keyword should not be used. Each argument can be specified directly as a value, e.g. 6 or 3.14159 or abc (a string of characters). The type of each argument is specified by the *format* keyword as explained below, so that Python will know how to interpret the value. If the word SELF is used for an argument it has a special meaning. A pointer is passed to the Python function which it converts into a reference to LAMMPS itself. This enables the function to call back to LAMMPS through its library interface as explained below. This allows the Python function to query or set values internal to LAMMPS which can affect the subsequent execution of the input script. A LAMMPS variable can also be used as an argument, specified as v_name, where "name" is the name of the variable. Any style of LAMMPS variable can be used, as defined by the *variable* command. Each time the Python function is invoked, the LAMMPS variable is evaluated and its value is passed to the Python function.

The *return* keyword is only needed if the Python function returns a value. The specified *varReturn* must be of the form v_name, where "name" is the name of a python-style LAMMPS variable, defined by the *variable* command. The Python function can return a numeric or string value, as specified by the *format* keyword.

As explained on the *variable* doc page, the definition of a python-style variable associates a Python function name with the variable. This must match the *func* setting for this command. For example these two commands would be self-consistent:

```
variable foo python myMultiply
python myMultiply return v_foo format f file funcs.py
```

The two commands can appear in either order in the input script so long as both are specified before the Python function is invoked for the first time.

The *format* keyword must be used if the *input* or *return* keyword is used. It defines an *fstring* with M characters, where M = sum of number of inputs and outputs. The order of characters corresponds to the N inputs, followed by the return value (if it exists). Each character must be one of the following: "i" for integer, "f" for floating point, "s" for string, or "p" for SELF. Each character defines the type of the corresponding input or output value of the Python function and affects the type conversion that is performed internally as data is passed back and forth between LAMMPS and Python. Note that it is permissible to use a *python-style variable* in a LAMMPS command that allows for an equal-style variable as an argument, but only if the output of the Python function is flagged as a numeric value ("i" or "f") via the *format* keyword.

If the *return* keyword is used and the *format* keyword specifies the output as a string, then the default maximum length of that string is 63 characters (64-1 for the string terminator). If you want to return a longer string, the *length* keyword can be specified with its *Nlen* value set to a larger number (the code allocates space for Nlen+1 to include the string terminator). If the Python function generates a string longer than the default 63 or the specified *Nlen*, it will be truncated.

Either the *file*, *here*, or *exists* keyword must be used, but only one of them. These keywords specify what Python code to load into the Python interpreter. The *file* keyword gives the name of a file, which should end with a ".py" suffix, which contains Python code. The code will be immediately loaded into and run in the "main" module of the Python interpreter. Note that Python code which contains a function definition does not "execute" the function when it is run; it simply defines the function so that it can be invoked later.

The *here* keyword does the same thing, except that the Python code follows as a single argument to the *here* keyword. This can be done using triple quotes as delimiters, as in the examples above. This allows Python code to be listed verbatim in your input script, with proper indentation, blank lines, and comments, as desired. See the *Commands parse* doc page, for an explanation of how triple quotes can be used as part of input script syntax.

The *exists* keyword takes no argument. It means that Python code containing the required Python function defined by the *func* setting, is assumed to have been previously loaded by another python command.

Note that the Python code that is loaded and run must contain a function with the specified *func* name. To operate properly when later invoked, the function code must match the *input* and *return* and *format* keywords specified by the python command. Otherwise Python will generate an error.

This section describes how Python code can be written to work with LAMMPS.

Whether you load Python code from a file or directly from your input script, via the *file* and *here* keywords, the code can be identical. It must be indented properly as Python requires. It can contain comments or blank lines. If the code is in your input script, it cannot however contain triple-quoted Python strings, since that will conflict with the triple-quote parsing that the LAMMPS input script performs.

All the Python code you specify via one or more python commands is loaded into the Python "main" module, i.e. __main__. The code can define global variables or statements that are outside of function definitions. It can contain multiple functions, only one of which matches the *func* setting in the python command. This means you can use the *file* keyword once to load several functions, and the *exists* keyword thereafter in subsequent python commands to access the other functions previously loaded.

A Python function you define (or more generally, the code you load) can import other Python modules or classes, it can make calls to other system functions or functions you define, and it can access or modify global variables (in the "main" module) which will persist between successive function calls. The latter can be useful, for example, to prevent a function from being invoke multiple times per timestep by different commands in a LAMMPS input script that access the returned python-style variable associated with the function. For example, consider this function loaded with two global variables defined outside the function:

```
nsteplast = -1
nvaluelast = 0

def expensive(nstep):
  global nsteplast,nvaluelast
  if nstep == nsteplast: return nvaluelast
  nsteplast = nstep
  # perform complicated calculation
  nvalue = ...
  nvaluelast = nvalue
  return nvalue
```

Nsteplast stores the previous timestep the function was invoked (passed as an argument to the function). Nvaluelast stores the return value computed on the last function invocation. If the function is invoked again on the same timestep, the previous value is simply returned, without re-computing it. The "global" statement inside the Python function allows it to overwrite the global variables.

Note that if you load Python code multiple times (via multiple python commands), you can overwrite previously loaded variables and functions if you are not careful. E.g. if the code above were loaded twice, the global variables would be re-initialized, which might not be what you want. Likewise, if a function with the same name exists in two chunks of Python code you load, the function loaded second will override the function loaded first.

It's important to realize that if you are running LAMMPS in parallel, each MPI task will load the Python interpreter and execute a local copy of the Python function(s) you define. There is no connection between the Python interpreters running on different processors. This implies three important things.

First, if you put a print statement in your Python function, you will see P copies of the output, when running on P processors. If the prints occur at (nearly) the same time, the P copies of the output may be mixed together. Welcome to the world of parallel programming and debugging.

Second, if your Python code loads modules that are not pre-loaded by the Python library, then it will load the module from disk. This may be a bottleneck if 1000s of processors try to load a module at the same time. On some large supercomputers, loading of modules from disk by Python may be disabled. In this case you would need to pre-build a Python library that has the required modules pre-loaded and link LAMMPS with that library.

Third, if your Python code calls back to LAMMPS (discussed in the next section) and causes LAMMPS to perform an MPI operation requires global communication (e.g. via MPI_Allreduce), such as computing the global temperature of the system, then you must insure all your Python functions (running independently on different processors) call back to LAMMPS. Otherwise the code may hang.

Your Python function can "call back" to LAMMPS through its library interface, if you use the SELF input to pass Python a pointer to LAMMPS. The mechanism for doing this in your Python function is as follows:

```
def foo(lmpptr,...):
  from lammps import lammps
  lmp = lammps(ptr=lmpptr)
  lmp.command('print "Hello from inside Python"')
  ...
```

The function definition must include a variable (lmpptr in this case) which corresponds to SELF in the python command. The first line of the function imports the Python module lammps.py in the python directory of the distribution. The second line creates a Python object "lmp" which wraps the instance of LAMMPS that called the function. The "ptr=lmpptr" argument is what makes that happen. The third line invokes the command() function in the LAMMPS library interface. It takes a single string argument which is a LAMMPS input script command for LAMMPS to execute, the same as if it appeared in your input script. In this case, LAMMPS should output

```
Hello from inside Python
```

to the screen and log file. Note that since the LAMMPS print command itself takes a string in quotes as its argument, the Python string must be delimited with a different style of quotes.

The *Python library* doc page describes the syntax for how Python wraps the various functions included in the LAMMPS library interface.

A more interesting example is in the examples/python/in.python script which loads and runs the following function from examples/python/funcs.py:

```
def loop(N,cut0,thresh,lmpptr):
  print "LOOP ARGS",N,cut0,thresh,lmpptr
  from lammps import lammps
  lmp = lammps(ptr=lmpptr)
  natoms = lmp.get_natoms()

  for i in range(N):
    cut = cut0 + i*0.1

    lmp.set_variable("cut",cut)                  # set a variable in LAMMPS
    lmp.command("pair_style lj/cut ${cut}")      # LAMMPS command
    #lmp.command("pair_style lj/cut %d" % cut)   # LAMMPS command option

    lmp.command("pair_coeff * * 1.0 1.0")        # ditto
    lmp.command("run 10")                        # ditto
    pe = lmp.extract_compute("thermo_pe",0,0)    # extract total PE from LAMMPS
    print "PE",pe/natoms,thresh
    if pe/natoms < thresh: return
```

with these input script commands:

```
python          loop input 4 10 1.0 -4.0 SELF format iffp file funcs.py
python          loop invoke
```

This has the effect of looping over a series of 10 short runs (10 timesteps each) where the pair style cutoff is increased from a value of 1.0 in distance units, in increments of 0.1. The looping stops when the per-atom potential energy falls below a threshold of -4.0 in energy units. More generally, Python can be used to implement a loop with complex logic, much more so than can be created using the LAMMPS *jump* and *if* commands.

Several LAMMPS library functions are called from the loop function. Get_natoms() returns the number of atoms in the simulation, so that it can be used to normalize the potential energy that is returned by extract_compute() for the "thermo_pe" compute that is defined by default for LAMMPS thermodynamic output. Set_variable() sets the value of a string variable defined in LAMMPS. This library function is a useful way for a Python function to return multiple values to LAMMPS, more than the single value that can be passed back via a return statement. This cutoff value in the "cut" variable is then substituted (by LAMMPS) in the pair_style command that is executed next. Alternatively, the "LAMMPS command option" line could be used in place of the 2 preceding lines, to have Python insert the value into the LAMMPS command string.

Note: When using the callback mechanism just described, recognize that there are some operations you should not attempt because LAMMPS cannot execute them correctly. If the Python function is invoked between runs in the LAMMPS input script, then it should be OK to invoke any LAMMPS input script command via the library interface command() or file() functions, so long as the command would work if it were executed in the LAMMPS input script directly at the same point.

However, a Python function can also be invoked during a run, whenever an associated LAMMPS variable it is assigned

to is evaluated. If the variable is an input argument to another LAMMPS command (e.g. *fix setforce*), then the Python function will be invoked inside the class for that command, in one of its methods that is invoked in the middle of a timestep. You cannot execute arbitrary input script commands from the Python function (again, via the command() or file() functions) at that point in the run and expect it to work. Other library functions such as those that invoke computes or other variables may have hidden side effects as well. In these cases, LAMMPS has no simple way to check that something illogical is being attempted.

The same applies to Python functions called during a simulation run at each time step using *fix python/invoke*.

If you run Python code directly on your workstation, either interactively or by using Python to launch a Python script stored in a file, and your code has an error, you will typically see informative error messages. That is not the case when you run Python code from LAMMPS using an embedded Python interpreter. The code will typically fail silently. LAMMPS will catch some errors but cannot tell you where in the Python code the problem occurred. For example, if the Python code cannot be loaded and run because it has syntax or other logic errors, you may get an error from Python pointing to the offending line, or you may get one of these generic errors from LAMMPS:

```
Could not process Python file
Could not process Python string
```

When the Python function is invoked, if it does not return properly, you will typically get this generic error from LAMMPS:

```
Python function evaluation failed
```

Here are three suggestions for debugging your Python code while running it under LAMMPS.

First, don't run it under LAMMPS, at least to start with! Debug it using plain Python. Load and invoke your function, pass it arguments, check return values, etc.

Second, add Python print statements to the function to check how far it gets and intermediate values it calculates. See the discussion above about printing from Python when running in parallel.

Third, use Python exception handling. For example, say this statement in your Python function is failing, because you have not initialized the variable foo:

```
foo += 1
```

If you put one (or more) statements inside a "try" statement, like this:

```
import exceptions
print "Inside simple function"
try:
  foo += 1      # one or more statements here
except Exception, e:
  print "FOO error:",e
```

then you will get this message printed to the screen:

```
FOO error: local variable 'foo' referenced before assignment
```

If there is no error in the try statements, then nothing is printed. Either way the function continues on (unless you put a return or sys.exit() in the except clause).

15.95.4 Restrictions

This command is part of the PYTHON package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Building LAMMPS with the PYTHON package will link LAMMPS with the Python library on your system. Settings to enable this are in the lib/python/Makefile.lammps file. See the lib/python/README file for information on those settings.

If you use Python code which calls back to LAMMPS, via the SELF input argument explained above, there is an extra step required when building LAMMPS. LAMMPS must also be built as a shared library and your Python function must be able to load the Python module in python/lammps.py that wraps the LAMMPS library interface. These are the same steps required to use Python by itself to wrap LAMMPS. Details on these steps are explained on the *Python* doc page. Note that it is important that the stand-alone LAMMPS executable and the LAMMPS shared library be consistent (built from the same source code files) in order for this to work. If the two have been built at different times using different source files, problems may occur.

15.95.5 Related commands

shell, *variable*, *fix python/invoke*

Default: none

15.96 quit command

15.96.1 Syntax

```
quit status
```

status = numerical exit status (optional)

15.96.2 Examples

```
quit
if "$n > 10000" then "quit 1"
```

15.96.3 Description

This command causes LAMMPS to exit, after shutting down all output cleanly.

It can be used as a debug statement in an input script, to terminate the script at some intermediate point.

It can also be used as an invoked command inside the "then" or "else" portion of an *if* command.

The optional status argument is an integer which signals the return status to a program calling LAMMPS. A return status of 0 usually indicates success. A status != 0 is failure, where the specified value can be used to distinguish the kind of error, e.g. where in the input script the quit was invoked. If not specified, a status of 0 is returned.

15.96.4 Restrictions

none

15.96.5 Related commands

if

Default: none

15.97 read_data command

15.97.1 Syntax

```
read_data file keyword args ...
```

- file = name of data file to read in
- zero or more keyword/arg pairs may be appended
- keyword = *add* or *offset* or *shift* or *extra/atom/types* or *extra/bond/types* or *extra/angle/types* or *extra/dihedral/types* or *extra/improper/types* or *extra/bond/per/atom* or *extra/angle/per/atom* or *extra/dihedral/per/atom* or *extra/improper/per/atom* or *group* or *nocoeff* or *fix*

```
add arg = append or IDoffset or IDoffset MOLoffset or merge
  append = add new atoms with atom IDs appended to current IDs
  IDoffset = add new atoms with atom IDs having IDoffset added
  MOLoffset = add new atoms with molecule IDs having MOLoffset added␣
↪(only when molecule IDs are enabled)
  merge = add new atoms with their atom IDs (and molecule IDs) unchanged
offset args = toff boff aoff doff ioff
  toff = offset to add to atom types
  boff = offset to add to bond types
  aoff = offset to add to angle types
  doff = offset to add to dihedral types
  ioff = offset to add to improper types
shift args = Sx Sy Sz
  Sx,Sy,Sz = distance to shift atoms when adding to system (distance␣
↪units)
extra/atom/types arg = # of extra atom types
extra/bond/types arg = # of extra bond types
extra/angle/types arg = # of extra angle types
extra/dihedral/types arg = # of extra dihedral types
extra/improper/types arg = # of extra improper types
extra/bond/per/atom arg = leave space for this many new bonds per atom
extra/angle/per/atom arg = leave space for this many new angles per atom
extra/dihedral/per/atom arg = leave space for this many new dihedrals per␣
↪atom
extra/improper/per/atom arg = leave space for this many new impropers per␣
↪atom
extra/special/per/atom arg = leave space for extra 1-2,1-3,1-4␣
↪interactions per atom
group args = groupID
```

```
    groupID = add atoms in data file to this group
  nocoeff = ignore force field parameters
  fix args = fix-ID header-string section-string
    fix-ID = ID of fix to process header lines and sections of data file
    header-string = header lines containing this string will be passed to␣
 ↪fix
    section-string = section names with this string will be passed to fix
```

15.97.2 Examples

```
read_data data.lj
read_data ../run7/data.polymer.gz
read_data data.protein fix mycmap crossterm CMAP
read_data data.water add append offset 3 1 1 1 1 shift 0.0 0.0 50.0
read_data data.water add merge 1 group solvent
```

15.97.3 Description

Read in a data file containing information LAMMPS needs to run a simulation. The file can be ASCII text or a gzipped text file (detected by a .gz suffix). This is one of 3 ways to specify initial atom coordinates; see the *read_restart* and *create_atoms* commands for alternative methods. Also see the explanation of the *-restart command-line switch* which can convert a restart file to a data file.

This command can be used multiple times to add new atoms and their properties to an existing system by using the *add*, *offset*, and *shift* keywords. See more details below, which includes the use case for the *extra* keywords.

The *group* keyword adds all the atoms in the data file to the specified group-ID. The group will be created if it does not already exist. This is useful if you are reading multiple data files and wish to put sets of atoms into different groups so they can be operated on later. E.g. a group of added atoms can be moved to new positions via the *displace_atoms* command. Note that atoms read from the data file are also always added to the "all" group. The *group* command discusses atom groups, as used in LAMMPS.

The *nocoeff* keyword tells read_data to ignore force field parameters. The various Coeff sections are still read and have to have the correct number of lines, but they are not applied. This also allows to read a data file without having any pair, bond, angle, dihedral or improper styles defined, or to read a data file for a different force field.

The use of the *fix* keyword is discussed below.

Reading multiple data files

The read_data command can be used multiple times with the same or different data files to build up a complex system from components contained in individual data files. For example one data file could contain fluid in a confined domain; a second could contain wall atoms, and the second file could be read a third time to create a wall on the other side of the fluid. The third set of atoms could be rotated to an opposing direction using the *displace_atoms* command, after the third read_data command is used.

The *add*, *offset*, *shift*, *extra*, and *group* keywords are useful in this context.

If a simulation box does not yet exist, the *add* keyword cannot be used; the read_data command is being used for the first time. If a simulation box does exist, due to using the *create_box* command, or a previous read_data command, then the *add* keyword must be used.

Note: The simulation box size (xlo to xhi, ylo to yhi, zlo to zhi) in the new data file will be merged with the existing simulation box to create a large enough box in each dimension to contain both the existing and new atoms. Each box

dimension never shrinks due to this merge operation, it only stays the same or grows. Care must be used if you are growing the existing simulation box in a periodic dimension. If there are existing atoms with bonds that straddle that periodic boundary, then the atoms may become far apart if the box size grows. This will separate the atoms in the bond, which can lead to "lost" bond atoms or bad dynamics.

The three choices for the *add* argument affect how the atom IDs and molecule IDs of atoms in the data file are treated. If *append* is specified, atoms in the data file are added to the current system, with their atom IDs reset so that an atom-ID = M in the data file becomes atom-ID = N+M, where N is the largest atom ID in the current system. This rule is applied to all occurrences of atom IDs in the data file, e.g. in the Velocity or Bonds section. This is also done for molecule IDs, if the atom style does support molecule IDs or they are enabled via fix property/atom. If *IDoffset* is specified, then *IDoffset* is a numeric value is given, e.g. 1000, so that an atom-ID = M in the data file becomes atom-ID = 1000+M. For systems with enabled molecule IDs, another numerical argument *MOLoffset* is required representing the equivalent offset for molecule IDs. If *merge* is specified, the data file atoms are added to the current system without changing their IDs. They are assumed to merge (without duplication) with the currently defined atoms. It is up to you to insure there are no multiply defined atom IDs, as LAMMPS only performs an incomplete check that this is the case by insuring the resulting max atom-ID >= the number of atoms. For molecule IDs, there is no check done at all.

The *offset* and *shift* keywords can only be used if the *add* keyword is also specified.

The *offset* keyword adds the specified offset values to the atom types, bond types, angle types, dihedral types, and improper types as they are read from the data file. E.g. if *toff* = 2, and the file uses atom types 1,2,3, then the added atoms will have atom types 3,4,5. These offsets apply to all occurrences of types in the data file, e.g. for the Atoms or Masses or Pair Coeffs or Bond Coeffs sections. This makes it easy to use atoms and molecules and their attributes from a data file in different simulations, where you want their types (atom, bond, angle, etc) to be different depending on what other types already exist. All five offset values must be specified, but individual values will be ignored if the data file does not use that attribute (e.g. no bonds).

The *shift* keyword can be used to specify an (Sx, Sy, Sz) displacement applied to the coordinates of each atom. Sz must be 0.0 for a 2d simulation. This is a mechanism for adding structured collections of atoms at different locations within the simulation box, to build up a complex geometry. It is up to you to insure atoms do not end up overlapping unphysically which would lead to bad dynamics. Note that the *displace_atoms* command can be used to move a subset of atoms after they have been read from a data file. Likewise, the *delete_atoms* command can be used to remove overlapping atoms. Note that the shift values (Sx, Sy, Sz) are also added to the simulation box information (xlo, xhi, ylo, yhi, zlo, zhi) in the data file to shift its boundaries. E.g. xlo_new = xlo + Sx, xhi_new = xhi + Sx.

The *extra* keywords can only be used the first time the read_data command is used. They are useful if you intend to add new atom, bond, angle, etc types later with additional read_data commands. This is because the maximum number of allowed atom, bond, angle, etc types is set by LAMMPS when the system is first initialized. If you do not use the *extra* keywords, then the number of these types will be limited to what appears in the first data file you read. For example, if the first data file is a solid substrate of Si, it will likely specify a single atom type. If you read a second data file with a different material (water molecules) that sit on top of the substrate, you will want to use different atom types for those atoms. You can only do this if you set the *extra/atom/types* keyword to a sufficiently large value when reading the substrate data file. Note that use of the *extra* keywords also allows each data file to contain sections like Masses or Pair Coeffs or Bond Coeffs which are sized appropriately for the number of types in that data file. If the *offset* keyword is used appropriately when each data file is read, the values in those sections will be stored correctly in the larger data structures allocated by the use of the *extra* keywords. E.g. the substrate file can list mass and pair coefficients for type 1 silicon atoms. The water file can list mass and pair coefficients for type 1 and type 2 hydrogen and oxygen atoms. Use of the *extra* and *offset* keywords will store those mass and pair coefficient values appropriately in data structures that allow for 3 atom types (Si, H, O). Of course, you would still need to specify coefficients for H/Si and O/Si interactions in your input script to have a complete pairwise interaction model.

An alternative to using the *extra* keywords with the read_data command, is to use the *create_box* command to initialize the simulation box and all the various type limits you need via its *extra* keywords. Then use the read_data command one or more times to populate the system with atoms, bonds, angles, etc, using the *offset* keyword if desired to alter types used in the various data files you read.

Format of a data file

The structure of the data file is important, though many settings and sections are optional or can come in any order. See the examples directory for sample data files for different problems.

A data file has a header and a body. The header appears first. The first line of the header is always skipped; it typically contains a description of the file. Then lines are read one at a time. Lines can have a trailing comment starting with '#' that is ignored. If the line is blank (only white-space after comment is deleted), it is skipped. If the line contains a header keyword, the corresponding value(s) is read from the line. If it doesn't contain a header keyword, the line begins the body of the file.

The body of the file contains zero or more sections. The first line of a section has only a keyword. This line can have a trailing comment starting with '#' that is either ignored or can be used to check for a style match, as described below. The next line is skipped. The remaining lines of the section contain values. The number of lines depends on the section keyword as described below. Zero or more blank lines can be used between sections. Sections can appear in any order, with a few exceptions as noted below.

The keyword *fix* can be used one or more times. Each usage specifies a fix that will be used to process a specific portion of the data file. Any header line containing *header-string* and any section with a name containing *section-string* will be passed to the specified fix. See the *fix property/atom* command for an example of a fix that operates in this manner. The doc page for the fix defines the syntax of the header line(s) and section(s) that it reads from the data file. Note that the *header-string* can be specified as NULL, in which case no header lines are passed to the fix. This means that it can infer the length of its Section from standard header settings, such as the number of atoms.

The formatting of individual lines in the data file (indentation, spacing between words and numbers) is not important except that header and section keywords (e.g. atoms, xlo xhi, Masses, Bond Coeffs) must be capitalized as shown and can't have extra white-space between their words - e.g. two spaces or a tab between the 2 words in "xlo xhi" or the 2 words in "Bond Coeffs", is not valid.

Format of the header of a data file

These are the recognized header keywords. Header lines can come in any order. The value(s) are read from the beginning of the line. Thus the keyword *atoms* should be in a line like "1000 atoms"; the keyword *ylo yhi* should be in a line like "-10.0 10.0 ylo yhi"; the keyword *xy xz yz* should be in a line like "0.0 5.0 6.0 xy xz yz". All these settings have a default value of 0, except the lo/hi box size defaults are -0.5 and 0.5. A line need only appear if the value is different than the default.

- *atoms* = # of atoms in system
- *bonds* = # of bonds in system
- *angles* = # of angles in system
- *dihedrals* = # of dihedrals in system
- *impropers* = # of impropers in system
- *atom types* = # of atom types in system
- *bond types* = # of bond types in system
- *angle types* = # of angle types in system
- *dihedral types* = # of dihedral types in system
- *improper types* = # of improper types in system
- *extra bond per atom* = leave space for this many new bonds per atom (deprecated, use extra/bond/per/atom keyword)
- *extra angle per atom* = leave space for this many new angles per atom (deprecated, use extra/angle/per/atom keyword)

- *extra dihedral per atom* = leave space for this many new dihedrals per atom (deprecated, use extra/dihedral/per/atom keyword)
- *extra improper per atom* = leave space for this many new impropers per atom (deprecated, use extra/improper/per/atom keyword)
- *extra special per atom* = leave space for this many new special bonds per atom (deprecated, use extra/special/per/atom keyword)
- *ellipsoids* = # of ellipsoids in system
- *lines* = # of line segments in system
- *triangles* = # of triangles in system
- *bodies* = # of bodies in system
- *xlo xhi* = simulation box boundaries in x dimension
- *ylo yhi* = simulation box boundaries in y dimension
- *zlo zhi* = simulation box boundaries in z dimension
- *xy xz yz* = simulation box tilt factors for triclinic system

The initial simulation box size is determined by the lo/hi settings. In any dimension, the system may be periodic or non-periodic; see the *boundary* command. When the simulation box is created it is also partitioned into a regular 3d grid of rectangular bricks, one per processor, based on the number of processors being used and the settings of the *processors* command. The partitioning can later be changed by the *balance* or *fix balance* commands.

If the *xy xz yz* line does not appear, LAMMPS will set up an axis-aligned (orthogonal) simulation box. If the line does appear, LAMMPS creates a non-orthogonal simulation domain shaped as a parallelepiped with triclinic symmetry. The parallelepiped has its "origin" at (xlo,ylo,zlo) and is defined by 3 edge vectors starting from the origin given by A = (xhi-xlo,0,0); B = (xy,yhi-ylo,0); C = (xz,yz,zhi-zlo). *Xy,xz,yz* can be 0.0 or positive or negative values and are called "tilt factors" because they are the amount of displacement applied to faces of an originally orthogonal box to transform it into the parallelepiped.

By default, the tilt factors (xy,xz,yz) can not skew the box more than half the distance of the corresponding parallel box length. For example, if xlo = 2 and xhi = 12, then the x box length is 10 and the xy tilt factor must be between -5 and 5. Similarly, both xz and yz must be between -(xhi-xlo)/2 and +(yhi-ylo)/2. Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = . . . , -15, -5, 5, 15, 25, . . . are all geometrically equivalent. If you wish to define a box with tilt factors that exceed these limits, you can use the *box tilt* command, with a setting of *large*; a setting of *small* is the default.

See the *Howto triclinic* doc page for a geometric description of triclinic boxes, as defined by LAMMPS, and how to transform these parameters to and from other commonly used triclinic representations.

When a triclinic system is used, the simulation domain should normally be periodic in the dimension that the tilt is applied to, which is given by the second dimension of the tilt factor (e.g. y for xy tilt). This is so that pairs of atoms interacting across that boundary will have one of them shifted by the tilt factor. Periodicity is set by the *boundary* command. For example, if the xy tilt factor is non-zero, then the y dimension should be periodic. Similarly, the z dimension should be periodic if xz or yz is non-zero. LAMMPS does not require this periodicity, but you may lose atoms if this is not the case.

Also note that if your simulation will tilt the box, e.g. via the *fix deform* command, the simulation box must be setup to be triclinic, even if the tilt factors are initially 0.0. You can also change an orthogonal box to a triclinic box or vice versa by using the *change box* command with its *ortho* and *triclinic* options.

For 2d simulations, the *zlo zhi* values should be set to bound the z coords for atoms that appear in the file; the default of -0.5 0.5 is valid if all z coords are 0.0. For 2d triclinic simulations, the xz and yz tilt factors must be 0.0.

If the system is periodic (in a dimension), then atom coordinates can be outside the bounds (in that dimension); they will be remapped (in a periodic sense) back inside the box. Note that if the *add* option is being used to add atoms to

a simulation box that already exists, this periodic remapping will be performed using simulation box bounds that are the union of the existing box and the box boundaries in the new data file.

Note: If the system is non-periodic (in a dimension), then all atoms in the data file must have coordinates (in that dimension) that are "greater than or equal to" the lo value and "less than or equal to" the hi value. If the non-periodic dimension is of style "fixed" (see the *boundary* command), then the atom coords must be strictly "less than" the hi value, due to the way LAMMPS assign atoms to processors. Note that you should not make the lo/hi values radically smaller/larger than the extent of the atoms. For example, if your atoms extend from 0 to 50, you should not specify the box bounds as -10000 and 10000. This is because LAMMPS uses the specified box size to layout the 3d grid of processors. A huge (mostly empty) box will be sub-optimal for performance when using "fixed" boundary conditions (see the *boundary* command). When using "shrink-wrap" boundary conditions (see the *boundary* command), a huge (mostly empty) box may cause a parallel simulation to lose atoms when LAMMPS shrink-wraps the box around the atoms. The read_data command will generate an error in this case.

The "extra bond per atom" setting (angle, dihedral, improper) is only needed if new bonds (angles, dihedrals, impropers) will be added to the system when a simulation runs, e.g. by using the *fix bond/create* command. Using this header flag is deprecated; please use the *extra/bond/per/atom* keyword (and correspondingly for angles, dihedrals and impropers) in the read_data command instead. Either will pre-allocate space in LAMMPS data structures for storing the new bonds (angles, dihedrals, impropers).

The "extra special per atom" setting is typically only needed if new bonds/angles/etc will be added to the system, e.g. by using the *fix bond/create* command. Or if entire new molecules will be added to the system, e.g. by using the *fix deposit* or *fix pour* commands, which will have more special 1-2,1-3,1-4 neighbors than any other molecules defined in the data file. Using this header flag is deprecated; please use the *extra/special/per/atom* keyword instead. Using this setting will pre-allocate space in the LAMMPS data structures for storing these neighbors. See the *special_bonds* and *molecule* doc pages for more discussion of 1-2,1-3,1-4 neighbors.

Note: All of the "extra" settings are only applied in the first data file read and when no simulation box has yet been created; as soon as the simulation box is created (and read_data implies that), these settings are *locked* and cannot be changed anymore. Please see the description of the *add* keyword above for reading multiple data files. If they appear in later data files, they are ignored.

The "ellipsoids" and "lines" and "triangles" and "bodies" settings are only used with *atom_style ellipsoid or line or tri or body* and specify how many of the atoms are finite-size ellipsoids or lines or triangles or bodies; the remainder are point particles. See the discussion of ellipsoidflag and the *Ellipsoids* section below. See the discussion of lineflag and the *Lines* section below. See the discussion of triangleflag and the *Triangles* section below. See the discussion of bodyflag and the *Bodies* section below.

Note: For *atom_style template*, the molecular topology (bonds,angles,etc) is contained in the molecule templates read-in by the *molecule* command. This means you cannot set the *bonds*, *angles*, etc header keywords in the data file, nor can you define *Bonds*, *Angles*, etc sections as discussed below. You can set the *bond types*, *angle types*, etc header keywords, though it is not necessary. If specified, they must match the maximum values defined in any of the template molecules.

Format of the body of a data file

These are the section keywords for the body of the file.

- *Atoms, Velocities, Masses, Ellipsoids, Lines, Triangles, Bodies* = atom-property sections
- *Bonds, Angles, Dihedrals, Impropers* = molecular topology sections

- *Pair Coeffs, PairIJ Coeffs, Bond Coeffs, Angle Coeffs, Dihedral Coeffs, Improper Coeffs* = force field sections
- *BondBond Coeffs, BondAngle Coeffs, MiddleBondTorsion Coeffs, EndBondTorsion Coeffs, AngleTorsion Coeffs, AngleAngleTorsion Coeffs, BondBond13 Coeffs, AngleAngle Coeffs* = class 2 force field sections

These keywords will check an appended comment for a match with the currently defined style:

- *Atoms, Pair Coeffs, PairIJ Coeffs, Bond Coeffs, Angle Coeffs, Dihedral Coeffs, Improper Coeffs*

For example, these lines:

```
Atoms # sphere
Pair Coeffs # lj/cut
```

will check if the currently-defined *atom_style* is *sphere*, and the current *pair_style* is *lj/cut*. If not, LAMMPS will issue a warning to indicate that the data file section likely does not contain the correct number or type of parameters expected for the currently-defined style.

Each section is listed below in alphabetic order. The format of each section is described including the number of lines it must contain and rules (if any) for where it can appear in the data file.

Any individual line in the various sections can have a trailing comment starting with "#" for annotation purposes. E.g. in the Atoms section:

```
10 1 17 -1.0 10.0 5.0 6.0   # salt ion
```

Angle Coeffs section:

- one line per angle type
- line syntax: ID coeffs

  ```
  ID = angle type (1-N)
  coeffs = list of coeffs
  ```

- example:

  ```
  6 70 108.5 0 0
  ```

The number and meaning of the coefficients are specific to the defined angle style. See the *angle_style* and *angle_coeff* commands for details. Coefficients can also be set via the *angle_coeff* command in the input script.

AngleAngle Coeffs section:

- one line per improper type
- line syntax: ID coeffs

  ```
  ID = improper type (1-N)
  coeffs = list of coeffs (see improper_coeff)
  ```

AngleAngleTorsion Coeffs section:

- one line per dihedral type
- line syntax: ID coeffs

  ```
  ID = dihedral type (1-N)
  coeffs = list of coeffs (see dihedral_coeff)
  ```

Angles section:

- one line per angle
- line syntax: ID type atom1 atom2 atom3

```
ID = number of angle (1-Nangles)
type = angle type (1-Nangletype)
atom1,atom2,atom3 = IDs of 1st,2nd,3rd atoms in angle
```

example:

```
2 2 17 29 430
```

The 3 atoms are ordered linearly within the angle. Thus the central atom (around which the angle is computed) is the atom2 in the list. E.g. H,O,H for a water molecule. The *Angles* section must appear after the *Atoms* section. All values in this section must be integers (1, not 1.0).

AngleTorsion Coeffs section:

- one line per dihedral type
- line syntax: ID coeffs

```
ID = dihedral type (1-N)
coeffs = list of coeffs (see dihedral_coeff)
```

Atoms section:

- one line per atom
- line syntax: depends on atom style

An *Atoms* section must appear in the data file if natoms > 0 in the header section. The atoms can be listed in any order. These are the line formats for each *atom style* in LAMMPS. As discussed below, each line can optionally have 3 flags (nx,ny,nz) appended to it, which indicate which image of a periodic simulation box the atom is in. These may be important to include for some kinds of analysis.

angle	atom-ID molecule-ID atom-type x y z
atomic	atom-ID atom-type x y z
body	atom-ID atom-type bodyflag mass x y z
bond	atom-ID molecule-ID atom-type x y z
charge	atom-ID atom-type q x y z
dipole	atom-ID atom-type q x y z mux muy muz
dpd	atom-ID atom-type theta x y z
edpd	atom-ID atom-type edpd_temp edpd_cv x y z
mdpd	atom-ID atom-type rho x y z
tdpd	atom-ID atom-type x y z cc1 cc2 . . . ccNspecies
electron	atom-ID atom-type q spin eradius x y z
ellipsoid	atom-ID atom-type ellipsoidflag density x y z
full	atom-ID molecule-ID atom-type q x y z
line	atom-ID molecule-ID atom-type lineflag density x y z
meso	atom-ID atom-type rho e cv x y z
molecular	atom-ID molecule-ID atom-type x y z
peri	atom-ID atom-type volume density x y z
smd	atom-ID atom-type molecule volume mass kernel-radius contact-radius x y z
sphere	atom-ID atom-type diameter density x y z
spin	atom-ID atom-type sp x y z spx spy spz
template	atom-ID molecule-ID template-index template-atom atom-type x y z
tri	atom-ID molecule-ID atom-type triangleflag density x y z
wavepacket	atom-ID atom-type charge spin eradius etag cs_re cs_im x y z
hybrid	atom-ID atom-type x y z sub-style1 sub-style2 . . .

The per-atom values have these meanings and units, listed alphabetically:

- atom-ID = integer ID of atom
- atom-type = type of atom (1-Ntype)
- bodyflag = 1 for body particles, 0 for point particles
- cc = chemical concentration for tDPD particles for each species (mole/volume units)
- contact-radius = ??? (distance units)
- cs_re,cs_im = real/imaginary parts of wave packet coefficients
- cv = heat capacity (need units) for SPH particles
- density = density of particle (mass/distance^3 or mass/distance^2 or mass/distance units, depending on dimensionality of particle)
- diameter = diameter of spherical atom (distance units)
- e = energy (need units) for SPH particles
- edpd_temp = temperature for eDPD particles (temperature units)
- edpd_cv = volumetric heat capacity for eDPD particles (energy/temperature/volume units)
- ellipsoidflag = 1 for ellipsoidal particles, 0 for point particles
- eradius = electron radius (or fixed-core radius)
- etag = integer ID of electron that each wave packet belongs to
- kernel-radius = ??? (distance units)
- lineflag = 1 for line segment particles, 0 for point or spherical particles

- mass = mass of particle (mass units)
- molecule-ID = integer ID of molecule the atom belongs to
- mux,muy,muz = components of dipole moment of atom (dipole units)
- q = charge on atom (charge units)
- rho = density (need units) for SPH particles
- spin = electron spin (+1/-1), 0 = nuclei, 2 = fixed-core, 3 = pseudo-cores (i.e. ECP)
- sp = norm of magnetic spin of atom (in number of Bohr magnetons)
- spx,spy,spz = components of magnetic spin of atom (adim normalized vector)
- template-atom = which atom within a template molecule the atom is
- template-index = which molecule within the molecule template the atom is part of
- theta = internal temperature of a DPD particle
- triangleflag = 1 for triangular particles, 0 for point or spherical particles
- volume = volume of Peridynamic particle (distance^3 units)
- x,y,z = coordinates of atom (distance units)

The units for these quantities depend on the unit style; see the *units* command for details.

For 2d simulations specify z as 0.0, or a value within the *zlo zhi* setting in the data file header.

The atom-ID is used to identify the atom throughout the simulation and in dump files. Normally, it is a unique value from 1 to Natoms for each atom. Unique values larger than Natoms can be used, but they will cause extra memory to be allocated on each processor, if an atom map array is used, but not if an atom map hash is used; see the *atom_modify* command for details. If an atom map is not used (e.g. an atomic system with no bonds), and you don't care if unique atom IDs appear in dump files, then the atom-IDs can all be set to 0.

The molecule ID is a 2nd identifier attached to an atom. Normally, it is a number from 1 to N, identifying which molecule the atom belongs to. It can be 0 if it is a non-bonded atom or if you don't care to keep track of molecule assignments.

The diameter specifies the size of a finite-size spherical particle. It can be set to 0.0, which means that atom is a point particle.

The ellipsoidflag, lineflag, triangleflag, and bodyflag determine whether the particle is a finite-size ellipsoid or line or triangle or body of finite size, or whether the particle is a point particle. Additional attributes must be defined for each ellipsoid, line, triangle, or body in the corresponding *Ellipsoids*, *Lines*, *Triangles*, or *Bodies* section.

The *template-index* and *template-atom* are only defined used by *atom_style template*. In this case the *molecule* command is used to define a molecule template which contains one or more molecules. If an atom belongs to one of those molecules, its *template-index* and *template-atom* are both set to positive integers; if not the values are both 0. The *template-index* is which molecule (1 to Nmols) the atom belongs to. The *template-atom* is which atom (1 to Natoms) within the molecule the atom is.

Some pair styles and fixes and computes that operate on finite-size particles allow for a mixture of finite-size and point particles. See the doc pages of individual commands for details.

For finite-size particles, the density is used in conjunction with the particle volume to set the mass of each particle as mass = density * volume. In this context, volume can be a 3d quantity (for spheres or ellipsoids), a 2d quantity (for triangles), or a 1d quantity (for line segments). If the volume is 0.0, meaning a point particle, then the density value is used as the mass. One exception is for the body atom style, in which case the mass of each particle (body or point particle) is specified explicitly. This is because the volume of the body is unknown.

Note that for 2d simulations of spheres, this command will treat them as spheres when converting density to mass. However, they can also be modeled as 2d discs (circles) if the *set density/disc* command is used to reset their mass after the read_data command is used. A *disc* keyword can also be used with time integration fixes, such as *fix nve/sphere* and *fix nvt/sphere* to time integrate their motion as 2d discs (not 3d spheres), by changing their moment of inertia.

For atom_style hybrid, following the 5 initial values (ID,type,x,y,z), specific values for each sub-style must be listed. The order of the sub-styles is the same as they were listed in the *atom_style* command. The sub-style specific values are those that are not the 5 standard ones (ID,type,x,y,z). For example, for the "charge" sub-style, a "q" value would appear. For the "full" sub-style, a "molecule-ID" and "q" would appear. These are listed in the same order they appear as listed above. Thus if

```
atom_style hybrid charge sphere
```

were used in the input script, each atom line would have these fields:

```
atom-ID atom-type x y z q diameter density
```

Note that if a non-standard value is defined by multiple sub-styles, it must appear multiple times in the atom line. E.g. the atom line for atom_style hybrid dipole full would list "q" twice:

```
atom-ID atom-type x y z q mux muy myz molecule-ID q
```

Atom lines specify the (x,y,z) coordinates of atoms. These can be inside or outside the simulation box. When the data file is read, LAMMPS wraps coordinates outside the box back into the box for dimensions that are periodic. As discussed above, if an atom is outside the box in a non-periodic dimension, it will be lost.

LAMMPS always stores atom coordinates as values which are inside the simulation box. It also stores 3 flags which indicate which image of the simulation box (in each dimension) the atom would be in if its coordinates were unwrapped across periodic boundaries. An image flag of 0 means the atom is still inside the box when unwrapped. A value of 2 means add 2 box lengths to get the unwrapped coordinate. A value of -1 means subtract 1 box length to get the unwrapped coordinate. LAMMPS updates these flags as atoms cross periodic boundaries during the simulation. The *dump* command can output atom coordinates in wrapped or unwrapped form, as well as the 3 image flags.

In the data file, atom lines (all lines or none of them) can optionally list 3 trailing integer values (nx,ny,nz), which are used to initialize the atom's image flags. If nx,ny,nz values are not listed in the data file, LAMMPS initializes them to 0. Note that the image flags are immediately updated if an atom's coordinates need to wrapped back into the simulation box.

It is only important to set image flags correctly in a data file if a simulation model relies on unwrapped coordinates for some calculation; otherwise they can be left unspecified. Examples of LAMMPS commands that use unwrapped coordinates internally are as follows:

- Atoms in a rigid body (see *fix rigid*, *fix rigid/small*) must have consistent image flags, so that when the atoms are unwrapped, they are near each other, i.e. as a single body.
- If the *replicate* command is used to generate a larger system, image flags must be consistent for bonded atoms when the bond crosses a periodic boundary. I.e. the values of the image flags should be different by 1 (in the appropriate dimension) for the two atoms in such a bond.
- If you plan to *dump* image flags and perform post-analysis that will unwrap atom coordinates, it may be important that a continued run (restarted from a data file) begins with image flags that are consistent with the previous run.

Note: If your system is an infinite periodic crystal with bonds then it is impossible to have fully consistent image flags. This is because some bonds will cross periodic boundaries and connect two atoms with the same image flag.

Atom velocities and other atom quantities not defined above are set to 0.0 when the *Atoms* section is read. Velocities can be set later by a *Velocities* section in the data file or by a *velocity* or *set* command in the input script.

Bodies section:

- one or more lines per body
- first line syntax: atom-ID Ninteger Ndouble

```
Ninteger = # of integer quantities for this particle
Ndouble = # of floating-point quantities for this particle
```

- 0 or more integer lines with total of Ninteger values
- 0 or more double lines with total of Ndouble values
- example:

```
12 3 6
2 3 2
1.0 2.0 3.0 1.0 2.0 4.0
```

- example:

```
12 0 14
1.0 2.0 3.0 1.0 2.0 4.0 1.0
2.0 3.0 1.0 2.0 4.0 4.0 2.0
```

The *Bodies* section must appear if *atom_style body* is used and any atoms listed in the *Atoms* section have a bodyflag = 1. The number of bodies should be specified in the header section via the "bodies" keyword.

Each body can have a variable number of integer and/or floating-point values. The number and meaning of the values is defined by the body style, as described in the *Howto body* doc page. The body style is given as an argument to the *atom_style body* command.

The Ninteger and Ndouble values determine how many integer and floating-point values are specified for this particle. Ninteger and Ndouble can be as large as needed and can be different for every body. Integer values are then listed next on subsequent lines. Lines are read one at a time until Ninteger values are read. Floating-point values follow on subsequent lines, Again lines are read one at a time until Ndouble values are read. Note that if there are no values of a particular type, no lines appear for that type.

The *Bodies* section must appear after the *Atoms* section.

Bond Coeffs section:

- one line per bond type
- line syntax: ID coeffs

```
ID = bond type (1-N)
coeffs = list of coeffs
```

- example:

```
4 250 1.49
```

The number and meaning of the coefficients are specific to the defined bond style. See the *bond_style* and *bond_coeff* commands for details. Coefficients can also be set via the *bond_coeff* command in the input script.

BondAngle Coeffs section:

- one line per angle type
- line syntax: ID coeffs

```
ID = angle type (1-N)
coeffs = list of coeffs (see class 2 section of angle_coeff)
```

BondBond Coeffs section:

- one line per angle type
- line syntax: ID coeffs

```
ID = angle type (1-N)
coeffs = list of coeffs (see class 2 section of angle_coeff)
```

BondBond13 Coeffs section:

- one line per dihedral type
- line syntax: ID coeffs

```
ID = dihedral type (1-N)
coeffs = list of coeffs (see class 2 section of dihedral_coeff)
```

Bonds section:

- one line per bond
- line syntax: ID type atom1 atom2

```
ID = bond number (1-Nbonds)
type = bond type (1-Nbondtype)
atom1,atom2 = IDs of 1st,2nd atoms in bond
```

- example:

```
12 3 17 29
```

The *Bonds* section must appear after the *Atoms* section. All values in this section must be integers (1, not 1.0).

Dihedral Coeffs section:

- one line per dihedral type
- line syntax: ID coeffs

```
ID = dihedral type (1-N)
coeffs = list of coeffs
```

- example:

```
3 0.6 1 0 1
```

The number and meaning of the coefficients are specific to the defined dihedral style. See the *dihedral_style* and *dihedral_coeff* commands for details. Coefficients can also be set via the *dihedral_coeff* command in the input script.

Dihedrals section:

- one line per dihedral
- line syntax: ID type atom1 atom2 atom3 atom4

```
ID = number of dihedral (1-Ndihedrals)
type = dihedral type (1-Ndihedraltype)
atom1,atom2,atom3,atom4 = IDs of 1st,2nd,3rd,4th atoms in dihedral
```

- example:

```
12 4 17 29 30 21
```

The 4 atoms are ordered linearly within the dihedral. The *Dihedrals* section must appear after the *Atoms* section. All values in this section must be integers (1, not 1.0).

Ellipsoids section:

- one line per ellipsoid
- line syntax: atom-ID shapex shapey shapez quatw quati quatj quatk

```
atom-ID = ID of atom which is an ellipsoid
shapex,shapey,shapez = 3 diameters of ellipsoid (distance units)
quatw,quati,quatj,quatk = quaternion components for orientation of atom
```

- example:

```
12 1 2 1 1 0 0 0
```

The *Ellipsoids* section must appear if *atom_style ellipsoid* is used and any atoms are listed in the *Atoms* section with an ellipsoidflag = 1. The number of ellipsoids should be specified in the header section via the "ellipsoids" keyword.

The 3 shape values specify the 3 diameters or aspect ratios of a finite-size ellipsoidal particle, when it is oriented along the 3 coordinate axes. They must all be non-zero values.

The values *quatw*, *quati*, *quatj*, and *quatk* set the orientation of the atom as a quaternion (4-vector). Note that the shape attributes specify the aspect ratios of an ellipsoidal particle, which is oriented by default with its x-axis along the simulation box's x-axis, and similarly for y and z. If this body is rotated (via the right-hand rule) by an angle theta around a unit vector (a,b,c), then the quaternion that represents its new orientation is given by (cos(theta/2), a*sin(theta/2), b*sin(theta/2), c*sin(theta/2)). These 4 components are quatw, quati, quatj, and quatk as specified above. LAMMPS normalizes each atom's quaternion in case (a,b,c) is not specified as a unit vector.

The *Ellipsoids* section must appear after the *Atoms* section.

EndBondTorsion Coeffs section:

- one line per dihedral type
- line syntax: ID coeffs

```
ID = dihedral type (1-N)
coeffs = list of coeffs (see class 2 section of dihedral_coeff)
```

Improper Coeffs section:

- one line per improper type
- line syntax: ID coeffs

```
ID = improper type (1-N)
coeffs = list of coeffs
```

- example:

```
2 20 0.0548311
```

The number and meaning of the coefficients are specific to the defined improper style. See the *improper_style* and *improper_coeff* commands for details. Coefficients can also be set via the *improper_coeff* command in the input script.

Impropers section:

- one line per improper
- line syntax: ID type atom1 atom2 atom3 atom4

```
ID = number of improper (1-Nimpropers)
type = improper type (1-Nimpropertype)
atom1,atom2,atom3,atom4 = IDs of 1st,2nd,3rd,4th atoms in improper
```

- example:

```
12 3 17 29 13 100
```

The ordering of the 4 atoms determines the definition of the improper angle used in the formula for each *improper style*. See the doc pages for individual styles for details.

The *Impropers* section must appear after the *Atoms* section. All values in this section must be integers (1, not 1.0).

Lines section:

- one line per line segment
- line syntax: atom-ID x1 y1 x2 y2

```
atom-ID = ID of atom which is a line segment
x1,y1 = 1st end point
x2,y2 = 2nd end point
```

- example:

```
12 1.0 0.0 2.0 0.0
```

The *Lines* section must appear if *atom_style line* is used and any atoms are listed in the *Atoms* section with a lineflag = 1. The number of lines should be specified in the header section via the "lines" keyword.

The 2 end points are the end points of the line segment. The ordering of the 2 points should be such that using a right-hand rule to cross the line segment with a unit vector in the +z direction, gives an "outward" normal vector

perpendicular to the line segment. I.e. normal = (c2-c1) x (0,0,1). This orientation may be important for defining some interactions.

The *Lines* section must appear after the *Atoms* section.

Masses section:

- one line per atom type
- line syntax: ID mass

```
ID = atom type (1-N)
mass = mass value
```

- example:

```
3 1.01
```

This defines the mass of each atom type. This can also be set via the *mass* command in the input script. This section cannot be used for atom styles that define a mass for individual atoms - e.g. *atom_style sphere*.

MiddleBondTorsion Coeffs section:

- one line per dihedral type
- line syntax: ID coeffs

```
ID = dihedral type (1-N)
coeffs = list of coeffs (see class 2 section of dihedral_coeff)
```

Pair Coeffs section:

- one line per atom type
- line syntax: ID coeffs

```
ID = atom type (1-N)
coeffs = list of coeffs
```

- example:

```
3 0.022 2.35197 0.022 2.35197
```

The number and meaning of the coefficients are specific to the defined pair style. See the *pair_style* and *pair_coeff* commands for details. Since pair coefficients for types I != J are not specified, these will be generated automatically by the pair style's mixing rule. See the individual pair_style doc pages and the *pair_modify mix* command for details. Pair coefficients can also be set via the *pair_coeff* command in the input script.

PairIJ Coeffs section:

- one line per pair of atom types for all I,J with I <= J
- line syntax: ID1 ID2 coeffs

```
ID1 = atom type I = 1-N
ID2 = atom type J = I-N, with I <= J
coeffs = list of coeffs
```

- examples:

```
3 3 0.022 2.35197 0.022 2.35197
3 5 0.022 2.35197 0.022 2.35197
```

This section must have N*(N+1)/2 lines where N = # of atom types. The number and meaning of the coefficients are specific to the defined pair style. See the *pair_style* and *pair_coeff* commands for details. Since pair coefficients for types I != J are all specified, these values will turn off the default mixing rule defined by the pair style. See the individual pair_style doc pages and the *pair_modify mix* command for details. Pair coefficients can also be set via the *pair_coeff* command in the input script.

Triangles section:

- one line per triangle
- line syntax: atom-ID x1 y1 z1 x2 y2 z2 x3 y3 z3

```
atom-ID = ID of atom which is a line segment
x1,y1,z1 = 1st corner point
x2,y2,z2 = 2nd corner point
x3,y3,z3 = 3rd corner point
```

- example:

```
12 0.0 0.0 0.0 2.0 0.0 1.0 0.0 2.0 1.0
```

The *Triangles* section must appear if *atom_style tri* is used and any atoms are listed in the *Atoms* section with a triangleflag = 1. The number of lines should be specified in the header section via the "triangles" keyword.

The 3 corner points are the corner points of the triangle. The ordering of the 3 points should be such that using a right-hand rule to go from point1 to point2 to point3 gives an "outward" normal vector to the face of the triangle. I.e. normal = (c2-c1) x (c3-c1). This orientation may be important for defining some interactions.

The *Triangles* section must appear after the *Atoms* section.

Velocities section:

- one line per atom
- line syntax: depends on atom style

all styles except those listed	atom-ID vx vy vz
electron	atom-ID vx vy vz ervel
ellipsoid	atom-ID vx vy vz lx ly lz
sphere	atom-ID vx vy vz wx wy wz
hybrid	atom-ID vx vy vz sub-style1 sub-style2 . . .

where the keywords have these meanings:

vx,vy,vz = translational velocity of atom lx,ly,lz = angular momentum of aspherical atom wx,wy,wz = angular velocity of spherical atom ervel = electron radial velocity (0 for fixed-core):ul

The velocity lines can appear in any order. This section can only be used after an *Atoms* section. This is because the *Atoms* section must have assigned a unique atom ID to each atom so that velocities can be assigned to them.

Vx, vy, vz, and ervel are in *units* of velocity. Lx, ly, lz are in units of angular momentum (distance-velocity-mass). Wx, Wy, Wz are in units of angular velocity (radians/time).

For atom_style hybrid, following the 4 initial values (ID,vx,vy,vz), specific values for each sub-style must be listed. The order of the sub-styles is the same as they were listed in the *atom_style* command. The sub-style specific values are those that are not the 5 standard ones (ID,vx,vy,vz). For example, for the "sphere" sub-style, "wx", "wy", "wz" values would appear. These are listed in the same order they appear as listed above. Thus if

```
atom_style hybrid electron sphere
```

were used in the input script, each velocity line would have these fields:

```
atom-ID vx vy vz ervel wx wy wz
```

Translational velocities can also be set by the *velocity* command in the input script.

15.97.4 Restrictions

To read gzipped data files, you must compile LAMMPS with the -DLAMMPS_GZIP option. See the *Build settings* doc page for details.

15.97.5 Related commands

read_dump, *read_restart*, *create_atoms*, *write_data*

15.97.6 Default

The default for all the *extra* keywords is 0.

15.98 read_dump command

15.98.1 Syntax

```
read_dump file Nstep field1 field2 ... keyword values ...
```

- file = name of dump file to read
- Nstep = snapshot timestep to read from file
- one or more fields may be appended

```
field = x or y or z or vx or vy or vz or q or ix or iy or iz or fx or fy␣
↪or fz
  x,y,z = atom coordinates
  vx,vy,vz = velocity components
  q = charge
  ix,iy,iz = image flags in each dimension
  fx,fy,fz = force components
```

- zero or more keyword/value pairs may be appended
- keyword = *nfile* or *box* or *replace* or *purge* or *trim* or *add* or *label* or *scaled* or *wrapped* or *format*

```
nfile value = Nfiles = how many parallel dump files exist
box value = yes or no = replace simulation box with dump box
replace value = yes or no = overwrite atoms with dump atoms
purge value = yes or no = delete all atoms before adding dump atoms
trim value = yes or no = trim atoms not in dump snapshot
add value = yes or keep or no = add new dump atoms to system
label value = field column
  field = one of the listed fields or id or type
  column = label on corresponding column in dump file
scaled value = yes or no = coords in dump file are scaled/unscaled
wrapped value = yes or no = coords in dump file are wrapped/unwrapped
format values = format of dump file, must be last keyword if used
  native = native LAMMPS dump file
  xyz = XYZ file
  adios [timeout value] = dump file written by the dump adios command
    timeout = specify waiting time for the arrival of the timestep when␣
↪running concurrently.
              The value is a float number and is interpreted in seconds.
  molfile style path = VMD molfile plugin interface
    style = dcd or xyz or others supported by molfile plugins
    path = optional path for location of molfile plugins
```

15.98.2 Examples

```
read_dump dump.file 5000 x y z
read_dump dump.xyz 5 x y z box no format xyz
read_dump dump.xyz 10 x y z box no format molfile xyz "../plugins"
read_dump dump.dcd 0 x y z box yes format molfile dcd
read_dump dump.file 1000 x y z vx vy vz box yes format molfile lammpstrj /usr/local/
↪lib/vmd/plugins/LINUXAMD64/plugins/molfile
read_dump dump.file 5000 x y vx vy trim yes
read_dump ../run7/dump.file.gz 10000 x y z box yes
read_dump dump.xyz 10 x y z box no format molfile xyz ../plugins
read_dump dump.dcd 0 x y z format molfile dcd
read_dump dump.file 1000 x y z vx vy vz format molfile lammpstrj /usr/local/lib/vmd/
↪plugins/LINUXAMD64/plugins/molfile
read_dump dump.bp 5000 x y z vx vy vz format adios
read_dump dump.bp 5000 x y z vx vy vz format adios timeout 60.0
```

15.98.3 Description

Read atom information from a dump file to overwrite the current atom coordinates, and optionally the atom velocities and image flags and the simulation box dimensions. This is useful for restarting a run from a particular snapshot in a dump file. See the *read_restart* and *read_data* commands for alternative methods to do this. Also see the *rerun* command for a means of reading multiple snapshots from a dump file.

Note that a simulation box must already be defined before using the read_dump command. This can be done by the *create_box*, *read_data*, or *read_restart* commands. The read_dump command can reset the simulation box dimensions, as explained below.

Also note that reading per-atom information from a dump snapshot is limited to the atom coordinates, velocities and image flags, as explained below. Other atom properties, which may be necessary to run a valid simulation, such as atom charge, or bond topology information for a molecular system, are not read from (or even contained in) dump files. Thus this auxiliary information should be defined in the usual way, e.g. in a data file read in by a *read_data* command, before using the read_dump command, or by the *set* command, after the dump snapshot is read.

If the dump filename specified as *file* ends with ".gz", the dump file is read in gzipped format. You cannot (yet) read a dump file that was written in binary format with a ".bin" suffix.

You can read dump files that were written (in parallel) to multiple files via the "%" wild-card character in the dump file name. If any specified dump file name contains a "%", they must all contain it. See the *dump* command for details. The "%" wild-card character is only supported by the *native* format for dump files, described next.

If reading parallel dump files, you must also use the *nfile* keyword to tell LAMMPS how many parallel files exist, via its specified *Nfiles* value.

The format of the dump file is selected through the *format* keyword. If specified, it must be the last keyword used, since all remaining arguments are passed on to the dump reader. The *native* format is for native LAMMPS dump files, written with a *dump atom* or *dump custom* command. The *xyz* format is for generic XYZ formatted dump files. These formats take no additional values.

The *molfile* format supports reading data through using the VMD molfile plugin interface. This dump reader format is only available, if the USER-MOLFILE package has been installed when compiling LAMMPS.

The *molfile* format takes one or two additional values. The *style* value determines the file format to be used and can be any format that the molfile plugins support, such as DCD or XYZ. Note that DCD dump files can be written by LAMMPS via the *dump dcd* command. The *path* value specifies a list of directories which LAMMPS will search for the molfile plugins appropriate to the specified *style*. The syntax of the *path* value is like other search paths: it can contain multiple directories separated by a colon (or semi-colon on windows). The *path* keyword is optional and defaults to ".", i.e. the current directory.

The *adios* format supports reading data that was written by the *dump adios* command. The entire dump is read in parallel across all the processes, dividing the atoms evenly among the processes. The number of writers that has written the dump file does not matter. Using the adios style for dump and read_dump is a convenient way to dump all atoms from *N* writers and read it back by *M* readers. If one is running two LAMMPS instances concurrently where one dumps data and the other is reading it with the rerun command, the timeout option can be specified to wait on the reader side for the arrival of the requested step.

Support for other dump format readers may be added in the future.

Global information is first read from the dump file, namely timestep and box information.

The dump file is scanned for a snapshot with a timestamp that matches the specified *Nstep*. This means the LAMMPS timestep the dump file snapshot was written on for the *native* or *adios* formats.

The list of timestamps available in an adios .bp file is stored in the variable *ntimestep*:

```
$ bpls dump.bp -d ntimestep
  uint64_t  ntimestep  5*scalar
    (0)    0 50 100 150 200
```

Note that the *xyz* and *molfile* formats do not store the timestep. For these formats, timesteps are numbered logically, in a sequential manner, starting from 0. Thus to access the 10th snapshot in an *xyz* or *mofile* formatted dump file, use *Nstep* = 9.

The dimensions of the simulation box for the selected snapshot are also read; see the *box* keyword discussion below. For the *native* format, an error is generated if the snapshot is for a triclinic box and the current simulation box is

orthogonal or vice versa. A warning will be generated if the snapshot box boundary conditions (periodic, shrink-wrapped, etc) do not match the current simulation boundary conditions, but the boundary condition information in the snapshot is otherwise ignored. See the "boundary" command for more details. The *adios* reader does the same as the *native* format reader.

For the *xyz* format, no information about the box is available, so you must set the *box* flag to *no*. See details below.

For the *molfile* format, reading simulation box information is typically supported, but the location of the simulation box origin is lost and no explicit information about periodicity or orthogonal/triclinic box shape is available. The USER-MOLFILE package makes a best effort to guess based on heuristics, but this may not always work perfectly.

Per-atom information from the dump file snapshot is then read from the dump file snapshot. This corresponds to the specified *fields* listed in the read_dump command. It is an error to specify a z-dimension field, namely *z*, *vz*, or *iz*, for a 2d simulation.

For dump files in *native* format, each column of per-atom data has a text label listed in the file. A matching label for each field must appear, e.g. the label "vy" for the field *vy*. For the *x*, *y*, *z* fields any of the following labels are considered a match:

```
x, xs, xu, xsu for field x
y, ys, yu, ysu for field y
z, zs, zu, zsu for field z
```

The meaning of xs (scaled), xu (unwrapped), and xsu (scaled and unwrapped) is explained on the *dump* command doc page. These labels are searched for in the list of column labels in the dump file, in order, until a match is found.

The dump file must also contain atom IDs, with a column label of "id".

If the *add* keyword is specified with a value of *yes* or *keep*, as discussed below, the dump file must contain atom types, with a column label of "type".

If a column label you want to read from the dump file is not a match to a specified field, the *label* keyword can be used to specify the specific column label from the dump file to associate with that field. An example is if a time-averaged coordinate is written to the dump file via the *fix ave/atom* command. The column will then have a label corresponding to the fix-ID rather than "x" or "xs". The *label* keyword can also be used to specify new column labels for fields *id* and *type*.

For dump files in *xyz* format, only the *x*, *y*, and *z* fields are supported. The dump file does not store atom IDs, so these are assigned consecutively to the atoms as they appear in the dump file, starting from 1. Thus you should insure that order of atoms is consistent from snapshot to snapshot in the XYZ dump file. See the *dump_modify sort* command if the XYZ dump file was written by LAMMPS.

For dump files in *molfile* format, the *x*, *y*, *z*, *vx*, *vy*, and *vz* fields can be specified. However, not all molfile formats store velocities, or their respective plugins may not support reading of velocities. The molfile dump files do not store atom IDs, so these are assigned consecutively to the atoms as they appear in the dump file, starting from 1. Thus you should insure that order of atoms are consistent from snapshot to snapshot in the molfile dump file. See the *dump_modify sort* command if the dump file was written by LAMMPS.

The *adios* format supports all fields that the *native* format supports except for the *q* charge field. The list of fields stored in an adios .bp file is recorded in the attributes *columns* (array of short strings) and *columnstr* (space-separated single string).

```
$ bpls -la dump.bp column*
  string    columns            attr   = {"id", "type", "x", "y", "z", "vx", "vy", "vz
↪"}
  string    columnstr          attr   = "id type x y z vx vy vz "
```

Information from the dump file snapshot is used to overwrite or replace properties of the current system. There are various options for how this is done, determined by the specified fields and optional keywords.

The timestep of the snapshot becomes the current timestep for the simulation. See the *reset_timestep* command if you wish to change this after the dump snapshot is read.

If the *box* keyword is specified with a *yes* value, then the current simulation box dimensions are replaced by the dump snapshot box dimensions. If the *box* keyword is specified with a *no* value, the current simulation box is unchanged.

If the *purge* keyword is specified with a *yes* value, then all current atoms in the system are deleted before any of the operations invoked by the *replace*, *trim*, or *add* keywords take place.

If the *replace* keyword is specified with a *yes* value, then atoms with IDs that are in both the current system and the dump snapshot have their properties overwritten by field values. If the *replace* keyword is specified with a *no* value, atoms with IDs that are in both the current system and the dump snapshot are not modified.

If the *trim* keyword is specified with a *yes* value, then atoms with IDs that are in the current system but not in the dump snapshot are deleted. These atoms are unaffected if the *trim* keyword is specified with a *no* value.

If the *add* keyword is specified with a *no* value (default), then dump file atoms with IDs that are not in the current system are not added to the system. They are simply ignored.

If a *yes* value is specified, the atoms with new IDs are added to the system but their atom IDs are not preserved. Instead, after all the atoms are added, new IDs are assigned to them in the same manner as is described for the *create_atoms* command. Basically the largest existing atom ID in the system is identified, and all the added atoms are assigned IDs that consecutively follow the largest ID.

If a *keep* value is specified, the atoms with new IDs are added to the system and their atom IDs are preserved. This may lead to non-contiguous IDs for the combined system.

Note that atoms added via the *add* keyword will only have the attributes read from the dump file due to the *field* arguments. For example, if *x* or *y* or *z* or *q* is not specified as a field, a value of 0.0 is used for added atoms. Added atoms must have an atom type, so this value must appear in the dump file.

Any other attributes (e.g. charge or particle diameter for spherical particles) will be set to default values, the same as if the *create_atoms* command were used.

Atom coordinates read from the dump file are first converted into unscaled coordinates, relative to the box dimensions of the snapshot. These coordinates are then be assigned to an existing or new atom in the current simulation. The coordinates will then be remapped to the simulation box, whether it is the original box or the dump snapshot box. If periodic boundary conditions apply, this means the atom will be remapped back into the simulation box if necessary. If shrink-wrap boundary conditions apply, the new coordinates may change the simulation box dimensions. If fixed boundary conditions apply, the atom will be lost if it is outside the simulation box.

For *native* format dump files, the 3 xyz image flags for an atom in the dump file are set to the corresponding values appearing in the dump file if the *ix*, *iy*, *iz* fields are specified. If not specified, the image flags for replaced atoms are not changed and image flags for new atoms are set to default values. If coordinates read from the dump file are in unwrapped format (e.g. *xu*) then the image flags for read-in atoms are also set to default values. The remapping procedure described in the previous paragraph will then change images flags for all atoms (old and new) if periodic boundary conditions are applied to remap an atom back into the simulation box.

Note: If you get a warning about inconsistent image flags after reading in a dump snapshot, it means one or more pairs of bonded atoms now have inconsistent image flags. As discussed on the *Errors common* doc page this may or may not cause problems for subsequent simulations. One way this can happen is if you read image flag fields from the dump file but do not also use the dump file box parameters.

LAMMPS knows how to compute unscaled and remapped coordinates for the snapshot column labels discussed above, e.g. *x*, *xs*, *xu*, *xsu*. If another column label is assigned to the *x* or *y* or *z* field via the *label* keyword, e.g. for coordinates

output by the *fix ave/atom* command, then LAMMPS needs to know whether the coordinate information in the dump file is scaled and/or wrapped. This can be set via the *scaled* and *wrapped* keywords. Note that the value of the *scaled* and *wrapped* keywords is ignored for fields *x* or *y* or *z* if the *label* keyword is not used to assign a column label to that field.

The scaled/unscaled and wrapped/unwrapped setting must be identical for any of the *x*, *y*, *z* fields that are specified. Thus you cannot read *xs* and *yu* from the dump file. Also, if the dump file coordinates are scaled and the simulation box is triclinic, then all 3 of the *x*, *y*, *z* fields must be specified, since they are all needed to generate absolute, unscaled coordinates.

15.98.4 Restrictions

To read gzipped dump files, you must compile LAMMPS with the -DLAMMPS_GZIP option. See the *Build settings* doc page for details.

The *molfile* dump file formats are part of the USER-MOLFILE package. They are only enabled if LAMMPS was built with that packages. See the *Build package* doc page for more info.

To write and read adios .bp files, you must compile LAMMPS with the *USER-ADIOS* package.

15.98.5 Related commands

dump, *dump molfile*, *dump adios*, *read_data*, *read_restart*, *rerun*

15.98.6 Default

The option defaults are box = yes, replace = yes, purge = no, trim = no, add = no, scaled = no, wrapped = yes, and format = native.

15.99 read_restart command

15.99.1 Syntax

```
read_restart file flag
```

- file = name of binary restart file to read in
- flag = remap (optional)

15.99.2 Examples

```
read_restart save.10000
read_restart save.10000 remap
read_restart restart.*
read_restart restart.*.mpiio
read_restart poly.*.% remap
```

15.99.3 Description

Read in a previously saved system configuration from a restart file. This allows continuation of a previous run. Details about what information is stored (and not stored) in a restart file is given below. Basically this operation will re-create the simulation box with all its atoms and their attributes as well as some related global settings, at the point in time it was written to the restart file by a previous simulation. The simulation box will be partitioned into a regular 3d grid of rectangular bricks, one per processor, based on the number of processors in the current simulation and the settings of the *processors* command. The partitioning can later be changed by the *balance* or *fix balance* commands.

Note: Normally, restart files are written by the *restart* or *write_restart* commands so that all atoms in the restart file are inside the simulation box. If this is not the case, the read_restart command will print an error that atoms were "lost" when the file is read. This error should be reported to the LAMMPS developers so the invalid writing of the restart file can be fixed. If you still wish to use the restart file, the optional *remap* flag can be appended to the read_restart command. This should avoid the error, by explicitly remapping each atom back into the simulation box, updating image flags for the atom appropriately.

Restart files are saved in binary format to enable exact restarts, meaning that the trajectories of a restarted run will precisely match those produced by the original run had it continued on.

Several things can prevent exact restarts due to round-off effects, in which case the trajectories in the 2 runs will slowly diverge. These include running on a different number of processors or changing certain settings such as those set by the *newton* or *processors* commands. LAMMPS will issue a warning in these cases.

Certain fixes will not restart exactly, though they should provide statistically similar results. These include *fix shake* and *fix langevin*.

Certain pair styles will not restart exactly, though they should provide statistically similar results. This is because the forces they compute depend on atom velocities, which are used at half-step values every timestep when forces are computed. When a run restarts, forces are initially evaluated with a full-step velocity, which is different than if the run had continued. These pair styles include *granular pair styles*, *pair dpd*, and *pair lubricate*.

If a restarted run is immediately different than the run which produced the restart file, it could be a LAMMPS bug, so consider *reporting it* if you think the behavior is a bug.

Because restart files are binary, they may not be portable to other machines. In this case, you can use the *-restart command-line switch* to convert a restart file to a data file.

Similar to how restart files are written (see the *write_restart* and *restart* commands), the restart filename can contain two wild-card characters. If a "*" appears in the filename, the directory is searched for all filenames that match the pattern where "*" is replaced with a timestep value. The file with the largest timestep value is read in. Thus, this effectively means, read the latest restart file. It's useful if you want your script to continue a run from where it left off. See the *run* command and its "upto" option for how to specify the run command so it doesn't need to be changed either.

If a "%" character appears in the restart filename, LAMMPS expects a set of multiple files to exist. The *restart* and *write_restart* commands explain how such sets are created. Read_restart will first read a filename where "%" is replaced by "base". This file tells LAMMPS how many processors created the set and how many files are in it. Read_restart then reads the additional files. For example, if the restart file was specified as save.% when it was written, then read_restart reads the files save.base, save.0, save.1, … save.P-1, where P is the number of processors that created the restart file.

Note that P could be the total number of processors in the previous simulation, or some subset of those processors, if the *fileper* or *nfile* options were used when the restart file was written; see the *restart* and *write_restart* commands for details. The processors in the current LAMMPS simulation share the work of reading these files; each reads a roughly equal subset of the files. The number of processors which created the set can be different the number of processors in the current LAMMPS simulation. This can be a fast mode of input on parallel machines that support parallel I/O.

A restart file can also be read in parallel as one large binary file via the MPI-IO library, assuming it was also written with MPI-IO. MPI-IO is part of the MPI standard for versions 2.0 and above. Using MPI-IO requires two steps. First, build LAMMPS with its MPIIO package installed, e.g.

```
make yes-mpiio    # installs the MPIIO package
make mpi          # build LAMMPS for your platform
```

Second, use a restart filename which contains ".mpiio". Note that it does not have to end in ".mpiio", just contain those characters. Unlike MPI-IO dump files, a particular restart file must be both written and read using MPI-IO.

Here is the list of information included in a restart file, which means these quantities do not need to be re-specified in the input script that reads the restart file, though you can redefine many of these settings after the restart file is read.

- *units*
- *newton bond* (see discussion of newton command below)
- *atom style* and *atom_modify* settings id, map, sort
- *comm style* and *comm_modify* settings mode, cutoff, vel
- *timestep*
- simulation box size and shape and *boundary* settings
- atom *group* definitions
- per-type atom settings such as *mass*
- per-atom attributes including their group assignments and molecular topology attributes (bonds, angles, etc)
- force field styles (*pair*, *bond*, *angle*, etc)
- force field coefficients (*pair*, *bond*, *angle*, etc) in some cases (see below)
- *pair_modify* settings, except the compute option
- *special_bonds* settings

Here is a list of information not stored in a restart file, which means you must re-issue these commands in your input script, after reading the restart file.

- *newton pair* (see discussion of newton command below)
- *fix* commands (see below)
- *compute* commands (see below)
- *variable* commands
- *region* commands
- *neighbor list* criteria including *neigh_modify* settings
- *kspace_style* and *kspace_modify* settings
- info for *thermodynamic*, *dump*, or *restart* output

The *newton* command has two settings, one for pairwise interactions, the other for bonded. Both settings are stored in the restart file. For the bond setting, the value in the file will overwrite the current value (at the time the read_restart command is issued) and warn if the two values are not the same and the current value is not the default. For the pair setting, the value in the file will not overwrite the current value (so that you can override the previous run's value), but a warning is issued if the two values are not the same and the current value is not the default.

Note that some force field styles (pair, bond, angle, etc) do not store their coefficient info in restart files. Typically these are many-body or tabulated potentials which read their parameters from separate files. In these cases you will need to re-specify the *pair_coeff*, *bond_coeff*, etc commands in your restart input script. The doc pages for individual force field styles mention if this is the case. This is also true of *pair_style hybrid* (bond hybrid, angle hybrid, etc) commands; they do not store coefficient info.

As indicated in the above list, the *fixes* used for a simulation are not stored in the restart file. This means the new input script should specify all fixes it will use. However, note that some fixes store an internal "state" which is written to the restart file. This allows the fix to continue on with its calculations in a restarted simulation. To re-enable such a fix, the fix command in the new input script must be of the same style and use the same fix-ID as was used in the input script that wrote the restart file.

If a match is found, LAMMPS prints a message indicating that the fix is being re-enabled. If no match is found before the first run or minimization is performed by the new script, the "state" information for the saved fix is discarded. At the time the discard occurs, LAMMPS will also print a list of fixes for which the information is being discarded. See the doc pages for individual fixes for info on which ones can be restarted in this manner. Note that fixes which are created internally by other LAMMPS commands (computes, fixes, etc) will have style names which are all-capitalized, and IDs which are generated internally.

Likewise, the *computes* used for a simulation are not stored in the restart file. This means the new input script should specify all computes it will use. However, some computes create a fix internally to store "state" information that persists from timestep to timestep. An example is the *compute msd* command which uses a fix to store a reference coordinate for each atom, so that a displacement can be calculated at any later time. If the compute command in the new input script uses the same compute-ID and group-ID as was used in the input script that wrote the restart file, then it will create the same fix in the restarted run. This means the re-created fix will be re-enabled with the stored state information as described in the previous paragraph, so that the compute can continue its calculations in a consistent manner.

Note: There are a handful of commands which can be used before or between runs which may require a system initialization. Examples include the "balance", "displace_atoms", "delete_atoms", "set" (some options), and "velocity" (some options) commands. This is because they can migrate atoms to new processors. Thus they will also discard unused "state" information from fixes. You will know the discard has occurred because a list of discarded fixes will be printed to the screen and log file, as explained above. This means that if you wish to retain that info in a restarted run, you must re-specify the relevant fixes and computes (which create fixes) before those commands are used.

Some pair styles, like the *granular pair styles*, also use a fix to store "state" information that persists from timestep to timestep. In the case of granular potentials, it is contact information between pairs of touching particles. This info will also be re-enabled in the restart script, assuming you re-use the same granular pair style.

LAMMPS allows bond interactions (angle, etc) to be turned off or deleted in various ways, which can affect how their info is stored in a restart file.

If bonds (angles, etc) have been turned off by the *fix shake* or *delete_bonds* command, their info will be written to a restart file as if they are turned on. This means they will need to be turned off again in a new run after the restart file is read.

Bonds that are broken (e.g. by a bond-breaking potential) are written to the restart file as broken bonds with a type of 0. Thus these bonds will still be broken when the restart file is read.

Bonds that have been broken by the *fix bond/break* command have disappeared from the system. No information about these bonds is written to the restart file.

15.99.4 Restrictions

To write and read restart files in parallel with MPI-IO, the MPIIO package must be installed.

15.99.5 Related commands

read_data, *read_dump*, *write_restart*, *restart*

Default: none

15.100 region command

15.100.1 Syntax

```
region ID style args keyword arg ...
```

- ID = user-assigned name for the region
- style = *delete* or *block* or *cone* or *cylinder* or *plane* or *prism* or *sphere* or *union* or *intersect*

```
delete = no args
block args = xlo xhi ylo yhi zlo zhi
  xlo,xhi,ylo,yhi,zlo,zhi = bounds of block in all dimensions (distance␣
↪units)
cone args = dim c1 c2 radlo radhi lo hi
  dim = x or y or z = axis of cone
  c1,c2 = coords of cone axis in other 2 dimensions (distance units)
  radlo,radhi = cone radii at lo and hi end (distance units)
  lo,hi = bounds of cone in dim (distance units)
cylinder args = dim c1 c2 radius lo hi
  dim = x or y or z = axis of cylinder
  c1,c2 = coords of cylinder axis in other 2 dimensions (distance units)
  radius = cylinder radius (distance units)
    c1,c2, and radius can be a variable (see below)
  lo,hi = bounds of cylinder in dim (distance units)
plane args = px py pz nx ny nz
  px,py,pz = point on the plane (distance units)
  nx,ny,nz = direction normal to plane (distance units)
prism args = xlo xhi ylo yhi zlo zhi xy xz yz
  xlo,xhi,ylo,yhi,zlo,zhi = bounds of untilted prism (distance units)
  xy = distance to tilt y in x direction (distance units)
  xz = distance to tilt z in x direction (distance units)
  yz = distance to tilt z in y direction (distance units)
sphere args = x y z radius
  x,y,z = center of sphere (distance units)
  radius = radius of sphere (distance units)
    x,y,z, and radius can be a variable (see below)
union args = N reg-ID1 reg-ID2 ...
  N = # of regions to follow, must be 2 or greater
  reg-ID1,reg-ID2, ... = IDs of regions to join together
intersect args = N reg-ID1 reg-ID2 ...
  N = # of regions to follow, must be 2 or greater
```

```
  reg-ID1,reg-ID2, ... = IDs of regions to intersect
```

- zero or more keyword/arg pairs may be appended
- keyword = *side* or *units* or *move* or *rotate* or *open*

```
side value = in or out
  in = the region is inside the specified geometry
  out = the region is outside the specified geometry
units value = lattice or box
  lattice = the geometry is defined in lattice units
  box = the geometry is defined in simulation box units
move args = v_x v_y v_z
  v_x,v_y,v_z = equal-style variables for x,y,z displacement of region␣
↪over time
rotate args = v_theta Px Py Pz Rx Ry Rz
  v_theta = equal-style variable for rotaton of region over time (in␣
↪radians)
  Px,Py,Pz = origin for axis of rotation (distance units)
  Rx,Ry,Rz = axis of rotation vector
open value = integer from 1-6 corresponding to face index (see below)
```

- accelerated styles (with same args) = *block/kk*

15.100.2 Examples

```
region 1 block -3.0 5.0 INF 10.0 INF INF
region 2 sphere 0.0 0.0 0.0 5 side out
region void cylinder y 2 3 5 -5.0 EDGE units box
region 1 prism 0 10 0 10 0 10 2 0 0
region outside union 4 side1 side2 side3 side4
region 2 sphere 0.0 0.0 0.0 5 side out move v_left v_up NULL
region openbox block 0 10 0 10 0 10 open 5 open 6 units box
region funnel cone z 10 10 2 5 0 10 open 1 units box
```

15.100.3 Description

This command defines a geometric region of space. Various other commands use regions. For example, the region can be filled with atoms via the *create_atoms* command. Or a bounding box around the region, can be used to define the simulation box via the *create_box* command. Or the atoms in the region can be identified as a group via the *group* command, or deleted via the *delete_atoms* command. Or the surface of the region can be used as a boundary wall via the *fix wall/region* command.

Commands which use regions typically test whether an atom's position is contained in the region or not. For this purpose, coordinates exactly on the region boundary are considered to be interior to the region. This means, for example, for a spherical region, an atom on the sphere surface would be part of the region if the sphere were defined with the *side in* keyword, but would not be part of the region if it were defined using the *side out* keyword. See more details on the *side* keyword below.

Normally, regions in LAMMPS are "static", meaning their geometric extent does not change with time. If the *move* or *rotate* keyword is used, as described below, the region becomes "dynamic", meaning it's location or orientation changes with time. This may be useful, for example, when thermostatting a region, via the compute temp/region command, or when the fix wall/region command uses a region surface as a bounding wall on particle motion, i.e. a rotating container.

The *delete* style removes the named region. Since there is little overhead to defining extra regions, there is normally no need to do this, unless you are defining and discarding large numbers of regions in your input script.

The lo/hi values for *block* or *cone* or *cylinder* or *prism* styles can be specified as EDGE or INF. EDGE means they extend all the way to the global simulation box boundary. Note that this is the current box boundary; if the box changes size during a simulation, the region does not. INF means a large negative or positive number (1.0e20), so it should encompass the simulation box even if it changes size. If a region is defined before the simulation box has been created (via *create_box* or *read_data* or *read_restart* commands), then an EDGE or INF parameter cannot be used. For a *prism* region, a non-zero tilt factor in any pair of dimensions cannot be used if both the lo/hi values in either of those dimensions are INF. E.g. if the xy tilt is non-zero, then xlo and xhi cannot both be INF, nor can ylo and yhi.

Note: Regions in LAMMPS do not get wrapped across periodic boundaries, as specified by the *boundary* command. For example, a spherical region that is defined so that it overlaps a periodic boundary is not treated as 2 half-spheres, one on either side of the simulation box.

Note: Regions in LAMMPS are always 3d geometric objects, regardless of whether the *dimension* of a simulation is 2d or 3d. Thus when using regions in a 2d simulation, you should be careful to define the region so that its intersection with the 2d x-y plane of the simulation has the 2d geometric extent you want.

For style *cone*, an axis-aligned cone is defined which is like a *cylinder* except that two different radii (one at each end) can be defined. Either of the radii (but not both) can be 0.0.

For style *cone* and *cylinder*, the c1,c2 params are coordinates in the 2 other dimensions besides the cylinder axis dimension. For dim = x, c1/c2 = y/z; for dim = y, c1/c2 = x/z; for dim = z, c1/c2 = x/y. Thus the third example above specifies a cylinder with its axis in the y-direction located at x = 2.0 and z = 3.0, with a radius of 5.0, and extending in the y-direction from -5.0 to the upper box boundary.

For style *plane*, a plane is defined which contain the point (px,py,pz) and has a normal vector (nx,ny,nz). The normal vector does not have to be of unit length. The "inside" of the plane is the half-space in the direction of the normal vector; see the discussion of the *side* option below.

For style *prism*, a parallelepiped is defined (it's too hard to spell parallelepiped in an input script!). The parallelepiped has its "origin" at (xlo,ylo,zlo) and is defined by 3 edge vectors starting from the origin given by A = (xhi-xlo,0,0); B = (xy,yhi-ylo,0); C = (xz,yz,zhi-zlo). *Xy,xz,yz* can be 0.0 or positive or negative values and are called "tilt factors" because they are the amount of displacement applied to faces of an originally orthogonal box to transform it into the parallelepiped.

A prism region that will be used with the *create_box* command to define a triclinic simulation box must have tilt factors (xy,xz,yz) that do not skew the box more than half the distance of corresponding the parallel box length. For example, if xlo = 2 and xhi = 12, then the x box length is 10 and the xy tilt factor must be between -5 and 5. Similarly, both xz and yz must be between -(xhi-xlo)/2 and +(yhi-ylo)/2. Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = ..., -15, -5, 5, 15, 25, ... are all geometrically equivalent.

The *radius* value for style *sphere* and *cylinder* can be specified as an equal-style *variable*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the radius of the region. For style *sphere* also the x-, y-, and z- coordinate of the center of the sphere and for style *cylinder* the two center positions c1 and c2 for the location of the cylinder axes can be a variable with the same kind of effect and requirements than for the radius.

Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent radius or have a time dependent position of the sphere or cylinder region.

See the *Howto tricilinc* doc page for a geometric description of triclinic boxes, as defined by LAMMPS, and how to transform these parameters to and from other commonly used triclinic representations.

The *union* style creates a region consisting of the volume of all the listed regions combined. The *intersect* style creates a region consisting of the volume that is common to all the listed regions.

Note: The *union* and *intersect* regions operate by invoking methods from their list of sub-regions. Thus you cannot delete the sub-regions after defining a *union* or *intersection* region.

The *side* keyword determines whether the region is considered to be inside or outside of the specified geometry. Using this keyword in conjunction with *union* and *intersect* regions, complex geometries can be built up. For example, if the interior of two spheres were each defined as regions, and a *union* style with *side* = out was constructed listing the region-IDs of the 2 spheres, the resulting region would be all the volume in the simulation box that was outside both of the spheres.

The *units* keyword determines the meaning of the distance units used to define the region for any argument above listed as having distance units. It also affects the scaling of the velocity vector specified with the *vel* keyword, the amplitude vector specified with the *wiggle* keyword, and the rotation point specified with the *rotate* keyword, since they each involve a distance metric.

A *box* value selects standard distance units as defined by the *units* command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacings which are used as follows:

- For style *block*, the lattice spacing in dimension x is applied to xlo and xhi, similarly the spacings in dimensions y,z are applied to ylo/yhi and zlo/zhi.
- For style *cone*, the lattice spacing in argument *dim* is applied to lo and hi. The spacings in the two radial dimensions are applied to c1 and c2. The two cone radii are scaled by the lattice spacing in the dimension corresponding to c1.
- For style *cylinder*, the lattice spacing in argument *dim* is applied to lo and hi. The spacings in the two radial dimensions are applied to c1 and c2. The cylinder radius is scaled by the lattice spacing in the dimension corresponding to c1.
- For style *plane*, the lattice spacing in dimension x is applied to px and nx, similarly the spacings in dimensions y,z are applied to py/ny and pz/nz.
- For style *prism*, the lattice spacing in dimension x is applied to xlo and xhi, similarly for ylo/yhi and zlo/zhi. The lattice spacing in dimension x is applied to xy and xz, and the spacing in dimension y to yz.
- For style *sphere*, the lattice spacing in dimensions x,y,z are applied to the sphere center x,y,z. The spacing in dimension x is applied to the sphere radius.

If the *move* or *rotate* keywords are used, the region is "dynamic", meaning its location or orientation changes with time. These keywords cannot be used with a *union* or *intersect* style region. Instead, the keywords should be used to make the individual sub-regions of the *union* or *intersect* region dynamic. Normally, each sub-region should be "dynamic" in the same manner (e.g. rotate around the same point), though this is not a requirement.

The *move* keyword allows one or more *equal-style variables* to be used to specify the x,y,z displacement of the region, typically as a function of time. A variable is specified as v_name, where name is the variable name. Any of the three variables can be specified as NULL, in which case no displacement is calculated in that dimension.

Note that equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a

region displacement that change as a function of time or spans consecutive runs in a continuous fashion. For the latter, see the *start* and *stop* keywords of the *run* command and the *elaplong* keyword of *thermo_style custom* for details.

For example, these commands would displace a region from its initial position, in the positive x direction, effectively at a constant velocity:

```
variable dx equal ramp(0,10)
region 2 sphere 10.0 10.0 0.0 5 move v_dx NULL NULL
```

Note that the initial displacement is 0.0, though that is not required.

Either of these variables would "wiggle" the region back and forth in the y direction:

```
variable dy equal swiggle(0,5,100)
variable dysame equal 5*sin(2*PI*elaplong*dt/100)
region 2 sphere 10.0 10.0 0.0 5 move NULL v_dy NULL
```

The *rotate* keyword rotates the region around a rotation axis *R* = (Rx,Ry,Rz) that goes through a point *P* = (Px,Py,Pz). The rotation angle is calculated, presumably as a function of time, by a variable specified as v_theta, where theta is the variable name. The variable should generate its result in radians. The direction of rotation for the region around the rotation axis is consistent with the right-hand rule: if your right-hand thumb points along *R*, then your fingers wrap around the axis in the direction of rotation.

The *move* and *rotate* keywords can be used together. In this case, the displacement specified by the *move* keyword is applied to the *P* point of the *rotate* keyword.

The *open* keyword can be used (multiple times) to indicate that one or more faces of the region are ignored for purposes of particle/wall interactions. This keyword is only relevant for regions used by the *fix wall/region* and *fix wall/gran/region* commands. It can be used to create "open" containers where only some of the region faces are walls. For example, a funnel can be created with a *cone* style region that has an open face at the smaller radius for particles to flow out, or at the larger radius for pouring particles into the cone, or both.

Note that using the *open* keyword partly overrides the *side* keyword, since both exterior and interior surfaces of an open region are tested for particle contacts. The exception to this is a *union* or *intersect* region which includes an open sub-region. In that case the *side* keyword is still used to define the union/intersect region volume, and the *open* settings are only applied to the individual sub-regions that use them.

The indices specified as part of the *open* keyword have the following meanings:

For style *block*, indices 1-6 correspond to the xlo, xhi, ylo, yhi, zlo, zhi surfaces of the block. I.e. 1 is the yz plane at x = xlo, 2 is the yz-plane at x = xhi, 3 is the xz plane at y = ylo, 4 is the xz plane at y = yhi, 5 is the xy plane at z = zlo, 6 is the xy plane at z = zhi). In the second-to-last example above, the region is a box open at both xy planes.

For style *prism*, values 1-6 have the same mapping as for style *block*. I.e. in an untilted *prism*, *open* indices correspond to the xlo, xhi, ylo, yhi, zlo, zhi surfaces.

For style *cylinder*, index 1 corresponds to the flat end cap at the low coordinate along the cylinder axis, index 2 corresponds to the high-coordinate flat end cap along the cylinder axis, and index 3 is the curved cylinder surface. For example, a *cylinder* region with *open 1 open 2* keywords will be open at both ends (e.g. a section of pipe), regardless of the cylinder orientation.

For style *cone*, the mapping is the same as for style *cylinder*. Index 1 is the low-coordinate flat end cap, index 2 is the high-coordinate flat end cap, and index 3 is the curved cone surface. In the last example above, a *cone* region is defined along the z-axis that is open at the zlo value (e.g. for use as a funnel).

For all other styles, the *open* keyword is ignored. As indicated above, this includes the *intersect* and *union* regions, though their sub-regions can be defined with the *open* keyword.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

The code using the region (such as a fix or compute) must also be supported by Kokkos or no acceleration will occur. Currently, only *block* style regions are supported by Kokkos.

These accelerated styles are part of the Kokkos package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

15.100.4 Restrictions

A prism cannot be of 0.0 thickness in any dimension; use a small z thickness for 2d simulations. For 2d simulations, the xz and yz parameters must be 0.0.

15.100.5 Related commands

lattice, *create_atoms*, *delete_atoms*, *group*

15.100.6 Default

The option defaults are side = in, units = lattice, and no move or rotation.

15.101 replicate command

15.101.1 Syntax

```
replicate nx ny nz keyword
```

nx,ny,nz = replication factors in each dimension

- optional *keyword* = *bbox*

  ```
  bbox = only check atoms in replicas that overlap with a processor's␣
  ↪sub-domain
  ```

15.101.2 Examples

```
replicate 2 3 2
```

15.101.3 Description

Replicate the current simulation one or more times in each dimension. For example, replication factors of 2,2,2 will create a simulation with 8x as many atoms by doubling the simulation domain in each dimension. A replication factor of 1 in a dimension leaves the simulation domain unchanged. When the new simulation box is created it is also partitioned into a regular 3d grid of rectangular bricks, one per processor, based on the number of processors being used and the settings of the *processors* command. The partitioning can later be changed by the *balance* or *fix balance* commands.

All properties of the atoms are replicated, including their velocities, which may or may not be desirable. New atom IDs are assigned to new atoms, as are molecule IDs. Bonds and other topology interactions are created between pairs of new atoms as well as between old and new atoms. This is done by using the image flag for each atom to "unwrap" it out of the periodic box before replicating it.

This means that any molecular bond you specify in the original data file that crosses a periodic boundary should be between two atoms with image flags that differ by 1. This will allow the bond to be unwrapped appropriately.

The optional keyword *bbox* uses a bounding box to only check atoms in replicas that overlap with a processor's sub-domain when assigning atoms to processors. It typically results in a substantial speedup when using the replicate command on a large number of processors. It does require temporary use of more memory, specifically that each processor can store all atoms in the entire system before it is replicated.

15.101.4 Restrictions

A 2d simulation cannot be replicated in the z dimension.

If a simulation is non-periodic in a dimension, care should be used when replicating it in that dimension, as it may put atoms nearly on top of each other.

Note: You cannot use the replicate command on a system which has a molecule that spans the box and is bonded to itself across a periodic boundary, so that the molecule is effectively a loop. A simple example would be a linear polymer chain that spans the simulation box and bonds back to itself across the periodic boundary. More realistic examples would be a CNT (meant to be an infinitely long CNT) or a graphene sheet or a bulk periodic crystal where there are explicit bonds specified between near neighbors. (Note that this only applies to systems that have permanent bonds as specified in the data file. A CNT that is just atoms modeled with the *AIREBO potential* has no such permanent bonds, so it can be replicated.) The reason replication does not work with those systems is that the image flag settings described above cannot be made consistent. I.e. it is not possible to define images flags so that when every pair of bonded atoms is unwrapped (using the image flags), they will be close to each other. The only way the replicate command could work in this scenario is for it to break a bond, insert more atoms, and re-connect the loop for the larger simulation box. But it is not clever enough to do this. So you will have to construct a larger version of your molecule as a pre-processing step and input a new data file to LAMMPS.

If the current simulation was read in from a restart file (before a run is performed), there must not be any fix information stored in the file for individual atoms. Similarly, no fixes can be defined at the time the replicate command is used that require vectors of atom information to be stored. This is because the replicate command does not know how to replicate that information for new atoms it creates. To work around this restriction, restart files may be converted into data files and fixes may be undefined via the *unfix* command before and redefined after the replicate command.

Related commands: none

Default: none

15.102 rerun command

15.102.1 Syntax

```
rerun file1 file2 ... keyword args ...
```

- file1,file2,... = dump file(s) to read
- one or more keywords may be appended, keyword *dump* must appear and be last

```
keyword = first or last or every or skip or start or stop or dump
 first args = Nfirst
   Nfirst = dump timestep to start on
 last args = Nlast
   Nlast = dumptimestep to stop on
 every args = Nevery
   Nevery = read snapshots matching every this many timesteps
 skip args = Nskip
   Nskip = read one out of every Nskip snapshots
 start args = Nstart
   Nstart = timestep on which pseudo run will start
 stop args = Nstop
   Nstop = timestep to which pseudo run will end
 dump args = same as read_dump command starting with its field arguments
```

15.102.2 Examples

```
rerun dump.file dump x y z vx vy vz
rerun dump1.txt dump2.txt first 10000 every 1000 dump x y z
rerun dump.vels dump x y z vx vy vz box yes format molfile lammpstrj
rerun dump.dcd dump x y z box no format molfile dcd
rerun ../run7/dump.file.gz skip 2 dump x y z box yes
rerun dump.bp dump x y z box no format adios
rerun dump.bp dump x y z vx vy vz format adios timeout 10.0
```

15.102.3 Description

Perform a pseudo simulation run where atom information is read one snapshot at a time from a dump file(s), and energies and forces are computed on the shapshot to produce thermodynamic or other output.

This can be useful in the following kinds of scenarios, after an initial simulation produced the dump file:

- Compute the energy and forces of snaphots using a different potential.
- Calculate one or more diagnostic quantities on the snapshots that weren't computed in the initial run. These can also be computed with settings not used in the initial run, e.g. computing an RDF via the *compute rdf* command with a longer cutoff than was used initially.
- Calculate the portion of per-atom forces resulting from a subset of the potential. E.g. compute only Coulombic forces. This can be done by only defining only a Coulombic pair style in the rerun script. Doing this in the original script would result in different (bad) dynamics.

Conceptually, using the rerun command is like running an input script that has a loop in it (see the *next* and *jump* commands). Each iteration of the loop reads one snapshot from the dump file via the *read_dump* command, sets the timestep to the appropriate value, and then invokes a *run* command for zero timesteps to simply compute energy and forces, and any other *thermodynamic output* or diagnostic info you have defined. This computation also invokes any fixes you have defined that apply constraints to the system, such as *fix shake* or *fix indent*.

Note that a simulation box must already be defined before using the rerun command. This can be done by the *create_box*, *read_data*, or *read_restart* commands.

Also note that reading per-atom information from dump snapshots is limited to the atom coordinates, velocities and image flags as explained in the *read_dump* command. Other atom properties, which may be necessary to compute energies and forces, such as atom charge, or bond topology information for a molecular system, are not read from (or even contained in) dump files. Thus this auxiliary information should be defined in the usual way, e.g. in a data file read in by a *read_data* command, before using the rerun command.

Also note that the frequency of thermodynamic or dump output from the rerun simulation will depend on settings made in the rerun script, the same as for output from any LAMMPS simulation. See further info below as to what that means if the timesteps for snapshots read from dump files do not match the specified output frequency.

If more than one dump file is specified, the dump files are read one after the other. It is assumed that snapshot timesteps will be in ascending order. If a snapshot is encountered that is not in ascending order, it will skip the snapshot until it reads one that is. This allows skipping of a duplicate snapshot (same timestep), e.g. that appeared at the end of one file and beginning of the next. However if you specify a series of dump files in an incorrect order (with respect to the timesteps they contain), you may skip large numbers of snapshots

Note that the dump files specified as part of the *dump* keyword can be parallel files, i.e. written as multiple files either per processor and/or per snapshot. If that is the case they will also be read in parallel which can make the rerun command operate dramatically faster for large systems. See the doc page for the *read_dump* and *dump* commands which describe how to read and write parallel dump files.

The *first*, *last*, *every*, *skip* keywords determine which snapshots are read from the dump file(s). Snapshots are skipped until they have a timestamp >= *Nfirst*. When a snapshot with a timestamp > *Nlast* is encountered, the rerun command finishes. Note below that the defaults for *first* and *last* are to read all snapshots. If the *every* keyword is set to a value > 0, then only snapshots with timestamps that are a multiple of *Nevery* are read (the first snapshot is always read). If *Nevery* = 0, then this criterion is ignored, i.e. every snapshot is read that meets the other criteria. If the *skip* keyword is used, then after the first snapshot is read, every Nth snapshot is read, where N = *Nskip*. E.g. if *Nskip* = 3, then only 1 out of every 3 snapshots is read, assuming the snapshot timestamp is also consistent with the other criteria.

The *start* and *stop* keywords do not affect which snapshots are read from the dump file(s). Rather, they have the same meaning that they do for the *run* command. They only need to be defined if (a) you are using a *fix* command that changes some value over time, and (b) you want the reference point for elapsed time (from start to stop) to be different than the *first* and *last* settings. See the doc page for individual fixes to see which ones can be used with the *start/stop* keywords. Note that if you define neither of the *start*/*stop* or *first*/*last* keywords, then LAMMPS treats the pseudo run as going from 0 to a huge value (effectively infinity). This means that any quantity that a fix scales as a fraction of elapsed time in the run, will essentially remain at its initial value. Also note that an error will occur if you read a snapshot from the dump file with a timestep value larger than the *stop* setting you have specified.

The *dump* keyword is required and must be the last keyword specified. Its arguments are passed internally to the *read_dump* command. The first argument following the *dump* keyword should be the *field1* argument of the *read_dump* command. See the *read_dump* doc page for details on the various options it allows for extracting information from the dump file snapshots, and for using that information to alter the LAMMPS simulation.

In general, a LAMMPS input script that uses a rerun command can include and perform all the usual operations of an input script that uses the *run* command. There are a few exceptions and points to consider, as discussed here.

Fixes that perform time integration, such as *fix nve* or *fix npt* are not invoked, since no time integration is performed. Fixes that perturb or constrain the forces on atoms will be invoked, just as they would during a normal run. Examples are *fix indent* and *fix langevin*. So you should think carefully as to whether that makes sense for the manner in which you are reprocessing the dump snapshots.

If you only want the rerun script to perform an analysis that does not involve pair interactions, such as use compute msd to calculated displacements over time, you do not need to define a *pair style*, which may also mean neighbor lists will not need to be calculated which saves time. The *comm_modify cutoff* command can also be used to insure ghost atoms are acquired from far enough away for operations like bond and angle evaluations, if no pair style is being used.

Every time a snapshot is read, the timestep for the simulation is reset, as if the *reset_timestep* command were used. This command has some restrictions as to what fixes can be defined. See its doc page for details. For example, the *fix deposit* and *fix dt/reset* fixes are in this category. They also make no sense to use with a rerun command.

If time-averaging fixes like *fix ave/time* are used, they are invoked on timesteps that are a function of their *Nevery*, *Nrepeat*, and *Nfreq* settings. As an example, see the *fix ave/time* doc page for details. You must insure those settings are consistent with the snapshot timestamps that are read from the dump file(s). If an averaging fix is not invoked on a timestep it expects to be, LAMMPS will flag an error.

The various forms of LAMMPS output, as defined by the *thermo_style*, *thermo*, *dump*, and *restart* commands occur with specified frequency, e.g. every N steps. If the timestep for a dump snapshot is not a multiple of N, then it will be read and processed, but no output will be produced. If you want output for every dump snapshot, you can simply use N=1 for an output frequency, e.g. for thermodynamic output or new dump file output.

15.102.4 Restrictions

To read gzipped dump files, you must compile LAMMPS with the -DLAMMPS_GZIP option. See the *Build settings* doc page for details.

15.102.5 Related commands

read_dump

15.102.6 Default

The option defaults are first = 0, last = a huge value (effectively infinity), start = same as first, stop = same as last, every = 0, skip = 1;

15.103 reset_ids command

15.103.1 Syntax

```
reset_ids
```

15.103.2 Examples

```
reset_ids
```

15.103.3 Description

Reset atom IDs for the system, including all the global IDs stored for bond, angle, dihedral, improper topology data. This will create a set of IDs that are numbered contiguously from 1 to N for a N atoms system.

This can be useful to do after performing a "delete_atoms" command for a molecular system. The delete_atoms compress yes option will not perform this operation due to the existence of bond topology. It can also be useful to do after any simulation which has lost atoms, e.g. due to atoms moving outside a simulation box with fixed boundaries (see the "boundary command"), or due to evaporation (see the "fix evaporate" command).

Note that the resetting of IDs is not really a compression, where gaps in atom IDs are removed by decrementing atom IDs that are larger. Instead the IDs for all atoms are erased, and new IDs are assigned so that the atoms owned by an individual processor have consecutive IDs, as the *create_atoms* command explains.

Note: If this command is used before a *pair style* is defined, an error about bond topology atom IDs not being found may result. This is because the cutoff distance for ghost atom communication was not sufficient to find atoms in bonds, angles, etc that are owned by other processors. The *comm_modify cutoff* command can be used to correct this issue. Or you can define a pair style before using this command. If you do the former, you should unset the comm_modify cutoff after using reset_ids so that subsequent communication is not inefficient.

15.103.4 Restrictions

none

15.103.5 Related commands

delete_atoms

Default: none

15.104 reset_timestep command

15.104.1 Syntax

```
reset_timestep N
```

- N = timestep number

15.104.2 Examples

```
reset_timestep 0
reset_timestep 4000000
```

15.104.3 Description

Set the timestep counter to the specified value. This command normally comes after the timestep has been set by reading a restart file via the *read_restart* command, or a previous simulation advanced the timestep.

The *read_data* and *create_box* commands set the timestep to 0; the *read_restart* command sets the timestep to the value it had when the restart file was written.

15.104.4 Restrictions

none

This command cannot be used when any fixes are defined that keep track of elapsed time to perform certain kinds of time-dependent operations. Examples are the *fix deposit* and *fix dt/reset* commands. The former adds atoms on specific timesteps. The latter keeps track of accumulated time.

Various fixes use the current timestep to calculate related quantities. If the timestep is reset, this may produce unexpected behavior, but LAMMPS allows the fixes to be defined even if the timestep is reset. For example, commands which thermostat the system, e.g. *fix nvt*, allow you to specify a target temperature which ramps from Tstart to Tstop which may persist over several runs. If you change the timestep, you may induce an instantaneous change in the target temperature.

Resetting the timestep clears flags for *computes* that may have calculated some quantity from a previous run. This means these quantity cannot be accessed by a variable in between runs until a new run is performed. See the *variable* command for more details.

15.104.5 Related commands

rerun

Default: none

15.105 restart command

15.105.1 Syntax

```
restart 0
restart N root keyword value ...
restart N file1 file2 keyword value ...
```

- N = write a restart file every this many timesteps
- N can be a variable (see below)
- root = filename to which timestep # is appended
- file1,file2 = two full filenames, toggle between them when writing file

- zero or more keyword/value pairs may be appended
- keyword = *fileper* or *nfile*

```
fileper arg = Np
  Np = write one file for every this many processors
nfile arg = Nf
  Nf = write this many files, one from each of Nf processors
```

15.105.2 Examples

```
restart 0
restart 1000 poly.restart
restart 1000 poly.restart.mpiio
restart 1000 restart.*.equil
restart 10000 poly.%.1 poly.%.2 nfile 10
restart v_mystep poly.restart
```

15.105.3 Description

Write out a binary restart file with the current state of the simulation every so many timesteps, in either or both of two modes, as a run proceeds. A value of 0 means do not write out any restart files. The two modes are as follows. If one filename is specified, a series of filenames will be created which include the timestep in the filename. If two filenames are specified, only 2 restart files will be created, with those names. LAMMPS will toggle between the 2 names as it writes successive restart files.

Note that you can specify the restart command twice, once with a single filename and once with two filenames. This would allow you, for example, to write out archival restart files every 100000 steps using a single filename, and more frequent temporary restart files every 1000 steps, using two filenames. Using restart 0 will turn off both modes of output.

Similar to *dump* files, the restart filename(s) can contain two wild-card characters.

If a "*" appears in the single filename, it is replaced with the current timestep value. This is only recognized when a single filename is used (not when toggling back and forth). Thus, the 3rd example above creates restart files as follows: restart.1000.equil, restart.2000.equil, etc. If a single filename is used with no "*", then the timestep value is appended. E.g. the 2nd example above creates restart files as follows: poly.restart.1000, poly.restart.2000, etc.

If a "%" character appears in the restart filename(s), then one file is written for each processor and the "%" character is replaced with the processor ID from 0 to P-1. An additional file with the "%" replaced by "base" is also written, which contains global information. For example, the files written on step 1000 for filename restart.% would be restart.base.1000, restart.0.1000, restart.1.1000, . . . , restart.P-1.1000. This creates smaller files and can be a fast mode of output and subsequent input on parallel machines that support parallel I/O. The optional *fileper* and *nfile* keywords discussed below can alter the number of files written.

The restart file can also be written in parallel as one large binary file via the MPI-IO library, which is part of the MPI standard for versions 2.0 and above. Using MPI-IO requires two steps. First, build LAMMPS with its MPIIO package installed, e.g.

```
make yes-mpiio     # installs the MPIIO package
make mpi           # build LAMMPS for your platform
```

Second, use a restart filename which contains ".mpiio". Note that it does not have to end in ".mpiio", just contain those characters. Unlike MPI-IO dump files, a particular restart file must be both written and read using MPI-IO.

Restart files are written on timesteps that are a multiple of N but not on the first timestep of a run or minimization. You can use the *write_restart* command to write a restart file before a run begins. A restart file is not written on the

last timestep of a run unless it is a multiple of N. A restart file is written on the last timestep of a minimization if N > 0 and the minimization converges.

Instead of a numeric value, N can be specified as an *equal-style variable*, which should be specified as v_name, where name is the variable name. In this case, the variable is evaluated at the beginning of a run to determine the next timestep at which a restart file will be written out. On that timestep, the variable will be evaluated again to determine the next timestep, etc. Thus the variable should return timestep values. See the stagger() and logfreq() and stride() math functions for *equal-style variables*, as examples of useful functions to use in this context. Other similar math functions could easily be added as options for *equal-style variables*.

For example, the following commands will write restart files every step from 1100 to 1200, and could be useful for debugging a simulation where something goes wrong at step 1163:

```
variable       s equal stride(1100,1200,1)
restart        v_s tmp.restart
```

See the *read_restart* command for information about what is stored in a restart file.

Restart files can be read by a *read_restart* command to restart a simulation from a particular state. Because the file is binary (to enable exact restarts), it may not be readable on another machine. In this case, you can use the *-r command-line switch* to convert a restart file to a data file.

Note: Although the purpose of restart files is to enable restarting a simulation from where it left off, not all information about a simulation is stored in the file. For example, the list of fixes that were specified during the initial run is not stored, which means the new input script must specify any fixes you want to use. Even when restart information is stored in the file, as it is for some fixes, commands may need to be re-specified in the new input script, in order to re-use that information. See the *read_restart* command for information about what is stored in a restart file.

The optional *nfile* or *fileper* keywords can be used in conjunction with the "%" wildcard character in the specified restart file name(s). As explained above, the "%" character causes the restart file to be written in pieces, one piece for each of P processors. By default P = the number of processors the simulation is running on. The *nfile* or *fileper* keyword can be used to set P to a smaller value, which can be more efficient when running on a large number of processors.

The *nfile* keyword sets P to the specified Nf value. For example, if Nf = 4, and the simulation is running on 100 processors, 4 files will be written, by processors 0,25,50,75. Each will collect information from itself and the next 24 processors and write it to a restart file.

For the *fileper* keyword, the specified value of Np means write one file for every Np processors. For example, if Np = 4, every 4th processor (0,4,8,12,etc) will collect information from itself and the next 3 processors and write it to a restart file.

15.105.4 Restrictions

To write and read restart files in parallel with MPI-IO, the MPIIO package must be installed.

15.105.5 Related commands

write_restart, *read_restart*

15.105.6 Default

```
restart 0
```

15.106 run command

15.106.1 Syntax

```
run N keyword values ...
```

- N = # of timesteps
- zero or more keyword/value pairs may be appended
- keyword = *upto* or *start* or *stop* or *pre* or *post* or *every*

```
upto value = none
start value = N1
  N1 = timestep at which 1st run started
stop value = N2
  N2 = timestep at which last run will end
pre value = no or yes
post value = no or yes
every values = M c1 c2 ...
  M = break the run into M-timestep segments and invoke one or more␣
↪commands between each segment
  c1,c2,...,cN = one or more LAMMPS commands, each enclosed in quotes
  c1 = NULL means no command will be invoked
```

15.106.2 Examples

```
run 10000
run 1000000 upto
run 100 start 0 stop 1000
run 1000 pre no post yes
run 100000 start 0 stop 1000000 every 1000 "print 'Protein Rg = $r'"
run 100000 every 1000 NULL
```

15.106.3 Description

Run or continue dynamics for a specified number of timesteps.

When the *run style* is *respa*, N refers to outer loop (largest) timesteps.

A value of N = 0 is acceptable; only the thermodynamics of the system are computed and printed without taking a timestep.

The *upto* keyword means to perform a run starting at the current timestep up to the specified timestep. E.g. if the current timestep is 10,000 and "run 100000 upto" is used, then an additional 90,000 timesteps will be run. This can be useful for very long runs on a machine that allocates chunks of time and terminate your job when time is exceeded. If you need to restart your script multiple times (reading in the last restart file), you can keep restarting your script with the same run command until the simulation finally completes.

The *start* or *stop* keywords can be used if multiple runs are being performed and you want a *fix* command that changes some value over time (e.g. temperature) to make the change across the entire set of runs and not just a single run. See the doc page for individual fixes to see which ones can be used with the *start/stop* keywords.

For example, consider this fix followed by 10 run commands:

```
fix         1 all nvt 200.0 300.0 1.0
run         1000 start 0 stop 10000
run         1000 start 0 stop 10000
...
run         1000 start 0 stop 10000
```

The NVT fix ramps the target temperature from 200.0 to 300.0 during a run. If the run commands did not have the start/stop keywords (just "run 1000"), then the temperature would ramp from 200.0 to 300.0 during the 1000 steps of each run. With the start/stop keywords, the ramping takes place over the 10000 steps of all runs together.

The *pre* and *post* keywords can be used to streamline the setup, clean-up, and associated output to the screen that happens before and after a run. This can be useful if you wish to do many short runs in succession (e.g. LAMMPS is being called as a library which is doing other computations between successive short LAMMPS runs).

By default (pre and post = yes), LAMMPS creates neighbor lists, computes forces, and imposes fix constraints before every run. And after every run it gathers and prints timings statistics. If a run is just a continuation of a previous run (i.e. no settings are changed), the initial computation is not necessary; the old neighbor list is still valid as are the forces. So if *pre* is specified as "no" then the initial setup is skipped, except for printing thermodynamic info. Note that if *pre* is set to "no" for the very 1st run LAMMPS performs, then it is overridden, since the initial setup computations must be done.

Note: If your input script changes the system between 2 runs, then the initial setup must be performed to insure the change is recognized by all parts of the code that are affected. Examples are adding a *fix* or *dump* or *compute*, changing a *neighbor* list parameter, or writing restart file which can migrate atoms between processors. LAMMPS has no easy way to check if this has happened, but it is an error to use the *pre no* option in this case.

If *post* is specified as "no", the full timing summary is skipped; only a one-line summary timing is printed.

The *every* keyword provides a means of breaking a LAMMPS run into a series of shorter runs. Optionally, one or more LAMMPS commands (c1, c2, . . . , cN) will be executed in between the short runs. If used, the *every* keyword must be the last keyword, since it has a variable number of arguments. Each of the trailing arguments is a single LAMMPS command, and each command should be enclosed in quotes, so that the entire command will be treated as a single argument. This will also prevent any variables in the command from being evaluated until it is executed multiple times during the run. Note that if a command itself needs one of its arguments quoted (e.g. the *print* command), then you can use a combination of single and double quotes, as in the example above or below.

The *every* keyword is a means to avoid listing a long series of runs and interleaving commands in your input script. For example, a *print* command could be invoked or a *fix* could be redefined, e.g. to reset a thermostat temperature. Or this could be useful for invoking a command you have added to LAMMPS that wraps some other code (e.g. as a library) to perform a computation periodically during a long LAMMPS run. See the *Modify* doc page for info about how to add new commands to LAMMPS. See the *Howto couple* doc page for ideas about how to couple LAMMPS to other codes.

With the *every* option, N total steps are simulated, in shorter runs of M steps each. After each M-length run, the specified commands are invoked. If only a single command is specified as NULL, then no command is invoked. Thus these lines:

```
variable q equal x[100]
run 6000 every 2000 "print 'Coord = $q'"
```

are the equivalent of:

```
variable q equal x[100]
run 2000
print "Coord = $q"
run 2000
print "Coord = $q"
run 2000
print "Coord = $q"
```

which does 3 runs of 2000 steps and prints the x-coordinate of a particular atom between runs. Note that the variable "$q" will be evaluated afresh each time the print command is executed.

Note that by using the line continuation character "&", the run every command can be spread across many lines, though it is still a single command:

```
run 100000 every 1000 &
  "print 'Minimum value = $a'" &
  "print 'Maximum value = $b'" &
  "print 'Temp = $c'" &
  "print 'Press = $d'"
```

If the *pre* and *post* options are set to "no" when used with the *every* keyword, then the 1st run will do the full setup and the last run will print the full timing summary, but these operations will be skipped for intermediate runs.

Note: You might wish to specify a command that exits the run by jumping out of the loop, e.g.

```
variable t equal temp
run 10000 every 100 "if '$t < 300.0' then 'jump SELF afterrun'"
```

However, this will not work. The run command simply executes each command one at a time each time it pauses, then continues the run.

Instead, you should use the *fix halt* command, which has additional options for how to exit the run.

15.106.4 Restrictions

When not using the *upto* keyword, the number of specified timesteps N must fit in a signed 32-bit integer, so you are limited to slightly more than 2 billion steps (2^31) in a single run. When using *upto*, N can be larger than a signed 32-bit integer, however the difference between N and the current timestep must still be no larger than 2^31 steps.

However, with or without the *upto* keyword, you can perform successive runs to run a simulation for any number of steps (ok, up to 2^63 total steps). I.e. the timestep counter within LAMMPS is a 64-bit signed integer.

15.106.5 Related commands

minimize, *run_style*, *temper*, *fix halt*

15.106.6 Default

The option defaults are start = the current timestep, stop = current timestep + N, pre = yes, and post = yes.

15.107 run_style command

15.107.1 Syntax

```
run_style style args
```

- style = *verlet* or *verlet/split* or *respa* or *respa/omp*

```
verlet args = none
verlet/split args = none
respa args = N n1 n2 ... keyword values ...
  N = # of levels of rRESPA
  n1, n2, ... = loop factors between rRESPA levels (N-1 values)
  zero or more keyword/value pairings may be appended to the loop factors
  keyword = bond or angle or dihedral or improper or
            pair or inner or middle or outer or hybrid or kspace
    bond value = M
      M = which level (1-N) to compute bond forces in
    angle value = M
      M = which level (1-N) to compute angle forces in
    dihedral value = M
      M = which level (1-N) to compute dihedral forces in
    improper value = M
      M = which level (1-N) to compute improper forces in
    pair value = M
      M = which level (1-N) to compute pair forces in
    inner values = M cut1 cut2
      M = which level (1-N) to compute pair inner forces in
      cut1 = inner cutoff between pair inner and
             pair middle or outer  (distance units)
      cut2 = outer cutoff between pair inner and
             pair middle or outer  (distance units)
    middle values = M cut1 cut2
      M = which level (1-N) to compute pair middle forces in
```

```
      cut1 = inner cutoff between pair middle and pair outer (distance␣
↪units)
      cut2 = outer cutoff between pair middle and pair outer (distance␣
↪units)
    outer value = M
      M = which level (1-N) to compute pair outer forces in
    hybrid values = M1 M2 ... (as many values as there are hybrid␣
↪sub-styles
      M1 = which level (1-N) to compute the first pair_style hybrid␣
↪sub-style in
      M2 = which level (1-N) to compute the second pair_style hybrid␣
↪sub-style in
      M3,etc
    kspace value = M
      M = which level (1-N) to compute kspace forces in
```

15.107.2 Examples

```
run_style verlet
run_style respa 4 2 2 2 bond 1 dihedral 2 pair 3 kspace 4
run_style respa 4 2 2 2 bond 1 dihedral 2 inner 3 5.0 6.0 outer 4 kspace 4
run_style respa 3 4 2 bond 1 hybrid 2 2 1 kspace 3
```

15.107.3 Description

Choose the style of time integrator used for molecular dynamics simulations performed by LAMMPS.

The *verlet* style is a standard velocity-Verlet integrator.

The *verlet/split* style is also a velocity-Verlet integrator, but it splits the force calculation within each timestep over 2 partitions of processors. See the *-partition command-line switch* for info on how to run LAMMPS with multiple partitions.

Specifically, this style performs all computation except the *kspace_style* portion of the force field on the 1st partition. This include the *pair style*, *bond style*, *neighbor list building*, *fixes* including time integration, and output. The *kspace_style* portion of the calculation is performed on the 2nd partition.

This is most useful for the PPPM kspace_style when its performance on a large number of processors degrades due to the cost of communication in its 3d FFTs. In this scenario, splitting your P total processors into 2 subsets of processors, P1 in the 1st partition and P2 in the 2nd partition, can enable your simulation to run faster. This is because the long-range forces in PPPM can be calculated at the same time as pair-wise and bonded forces are being calculated, and the FFTs can actually speed up when running on fewer processors.

To use this style, you must define 2 partitions where P1 is a multiple of P2. Typically having P1 be 3x larger than P2 is a good choice. The 3d processor layouts in each partition must overlay in the following sense. If P1 is a Px1 by Py1 by Pz1 grid, and P2 = Px2 by Py2 by Pz2, then Px1 must be an integer multiple of Px2, and similarly for Py1 a multiple of Py2, and Pz1 a multiple of Pz2.

Typically the best way to do this is to let the 1st partition choose its onn optimal layout, then require the 2nd partition's layout to match the integer multiple constraint. See the *processors* command with its *part* keyword for a way to control this, e.g.

```
processors * * * part 1 2 multiple
```

You can also use the *partition* command to explicitly specify the processor layout on each partition. E.g. for 2 partitions of 60 and 15 processors each:

```
partition yes 1 processors 3 4 5
partition yes 2 processors 3 1 5
```

When you run in 2-partition mode with the *verlet/split* style, the thermodynamic data for the entire simulation will be output to the log and screen file of the 1st partition, which are log.lammps.0 and screen.0 by default; see the *-plog and -pscreen command-line switches* to change this. The log and screen file for the 2nd partition will not contain thermodynamic output beyond the 1st timestep of the run.

See the *Speed packages* doc page for performance details of the speed-up offered by the *verlet/split* style. One important performance consideration is the assignment of logical processors in the 2 partitions to the physical cores of a parallel machine. The *processors* command has options to support this, and strategies are discussed in *Section 5* of the manual.

The *respa* style implements the rRESPA multi-timescale integrator *(Tuckerman)* with N hierarchical levels, where level 1 is the innermost loop (shortest timestep) and level N is the outermost loop (largest timestep). The loop factor arguments specify what the looping factor is between levels. N1 specifies the number of iterations of level 1 for a single iteration of level 2, N2 is the iterations of level 2 per iteration of level 3, etc. N-1 looping parameters must be specified.

Thus with a 4-level respa setting of "2 2 2" for the 3 loop factors, you could choose to have bond interactions computed 8x per large timestep, angle interactions computed 4x, pair interactions computed 2x, and long-range interactions once per large timestep.

The *timestep* command sets the large timestep for the outermost rRESPA level. Thus if the 3 loop factors are "2 2 2" for 4-level rRESPA, and the outer timestep is set to 4.0 fmsec, then the inner timestep would be 8x smaller or 0.5 fmsec. All other LAMMPS commands that specify number of timesteps (e.g. *thermo* for thermo output every N steps, *neigh_modify delay/every* parameters, *dump* every N steps, etc) refer to the outermost timesteps.

The rRESPA keywords enable you to specify at what level of the hierarchy various forces will be computed. If not specified, the defaults are that bond forces are computed at level 1 (innermost loop), angle forces are computed where bond forces are, dihedral forces are computed where angle forces are, improper forces are computed where dihedral forces are, pair forces are computed at the outermost level, and kspace forces are computed where pair forces are. The inner, middle, outer forces have no defaults.

For fixes that support it, the rRESPA level at which a given fix is active, can be selected through the *fix_modify* command.

The *inner* and *middle* keywords take additional arguments for cutoffs that are used by the pairwise force computations. If the 2 cutoffs for *inner* are 5.0 and 6.0, this means that all pairs up to 6.0 apart are computed by the inner force. Those between 5.0 and 6.0 have their force go ramped to 0.0 so the overlap with the next regime (middle or outer) is smooth. The next regime (middle or outer) will compute forces for all pairs from 5.0 outward, with those from 5.0 to 6.0 having their value ramped in an inverse manner.

Note that you can use *inner* and *outer* without using *middle* to split the pairwise computations into two portions instead of three. Unless you are using a very long pairwise cutoff, a 2-way split is often faster than a 3-way split, since it avoids too much duplicate computation of pairwise interactions near the intermediate cutoffs.

Also note that only a few pair potentials support the use of the *inner* and *middle* and *outer* keywords. If not, only the *pair* keyword can be used with that pair style, meaning all pairwise forces are computed at the same rRESPA level. See the doc pages for individual pair styles for details.

Another option for using pair potentials with rRESPA is with the *hybrid* keyword, which requires the use of the *pair_style hybrid or hybrid/overlay* command. In this scenario, different sub-styles of the hybrid pair style are

evaluated at different rRESPA levels. This can be useful, for example, to set different timesteps for hybrid coarse-grained/all-atom models. The *hybrid* keyword requires as many level assignments as there are hybrid sub-styles, which assigns each sub-style to a rRESPA level, following their order of definition in the pair_style command. Since the *hybrid* keyword operates on pair style computations, it is mutually exclusive with either the *pair* or the *inner*/*middle*/*outer* keywords.

When using rRESPA (or for any MD simulation) care must be taken to choose a timestep size(s) that insures the Hamiltonian for the chosen ensemble is conserved. For the constant NVE ensemble, total energy must be conserved. Unfortunately, it is difficult to know *a priori* how well energy will be conserved, and a fairly long test simulation (~10 ps) is usually necessary in order to verify that no long-term drift in energy occurs with the trial set of parameters.

With that caveat, a few rules-of-thumb may be useful in selecting *respa* settings. The following applies mostly to biomolecular simulations using the CHARMM or a similar all-atom force field, but the concepts are adaptable to other problems. Without SHAKE, bonds involving hydrogen atoms exhibit high-frequency vibrations and require a timestep on the order of 0.5 fmsec in order to conserve energy. The relatively inexpensive force computations for the bonds, angles, impropers, and dihedrals can be computed on this innermost 0.5 fmsec step. The outermost timestep cannot be greater than 4.0 fmsec without risking energy drift. Smooth switching of forces between the levels of the rRESPA hierarchy is also necessary to avoid drift, and a 1-2 angstrom "healing distance" (the distance between the outer and inner cutoffs) works reasonably well. We thus recommend the following settings for use of the *respa* style without SHAKE in biomolecular simulations:

```
timestep  4.0
run_style respa 4 2 2 2 inner 2 4.5 6.0 middle 3 8.0 10.0 outer 4
```

With these settings, users can expect good energy conservation and roughly a 2.5 fold speedup over the *verlet* style with a 0.5 fmsec timestep.

If SHAKE is used with the *respa* style, time reversibility is lost, but substantially longer time steps can be achieved. For biomolecular simulations using the CHARMM or similar all-atom force field, bonds involving hydrogen atoms exhibit high frequency vibrations and require a time step on the order of 0.5 fmsec in order to conserve energy. These high frequency modes also limit the outer time step sizes since the modes are coupled. It is therefore desirable to use SHAKE with respa in order to freeze out these high frequency motions and increase the size of the time steps in the respa hierarchy. The following settings can be used for biomolecular simulations with SHAKE and rRESPA:

```
fix             2 all shake 0.000001 500 0 m 1.0 a 1
timestep        4.0
run_style       respa 2 2 inner 1 4.0 5.0 outer 2
```

With these settings, users can expect good energy conservation and roughly a 1.5 fold speedup over the *verlet* style with SHAKE and a 2.0 fmsec timestep.

For non-biomolecular simulations, the *respa* style can be advantageous if there is a clear separation of time scales - fast and slow modes in the simulation. For example, a system of slowly-moving charged polymer chains could be setup as follows:

```
timestep 4.0
run_style respa 2 8
```

This is two-level rRESPA with an 8x difference between the short and long timesteps. The bonds, angles, dihedrals will be computed every 0.5 fs (assuming real units), while the pair and kspace interactions will be computed once every 4 fs. These are the default settings for each kind of interaction, so no additional keywords are necessary.

Even a LJ system can benefit from rRESPA if the interactions are divided by the inner, middle and outer keywords. A 2-fold or more speedup can be obtained while maintaining good energy conservation. In real units, for a pure LJ fluid at liquid density, with a sigma of 3.0 angstroms, and epsilon of 0.1 Kcal/mol, the following settings seem to work well:

```
timestep  36.0
run_style respa 3 3 4 inner 1 3.0 4.0 middle 2 6.0 7.0 outer 3
```

The *respa/omp* style is a variant of *respa* adapted for use with pair, bond, angle, dihedral, improper, or kspace styles with an *omp* suffix. It is functionally equivalent to *respa* but performs additional operations required for managing *omp* styles. For more on *omp* styles see the *Speed omp* doc page. Accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

You can specify *respa/omp* explicitly in your input script, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

15.107.4 Restrictions

The *verlet/split* style can only be used if LAMMPS was built with the REPLICA package. Correspondingly the *respa/omp* style is available only if the USER-OMP package was included. See the *Build package* doc page for more info.

Whenever using rRESPA, the user should experiment with trade-offs in speed and accuracy for their system, and verify that they are conserving energy to adequate precision.

15.107.5 Related commands

timestep, *run*

15.107.6 Default

```
run_style verlet
```

For run_style respa, the default assignment of interactions to rRESPA levels is as follows:

- bond forces = level 1 (innermost loop)
- angle forces = same level as bond forces
- dihedral forces = same level as angle forces
- improper forces = same level as dihedral forces
- pair forces = level N (outermost level)
- kspace forces = same level as pair forces
- inner, middle, outer forces = no default

(Tuckerman) Tuckerman, Berne and Martyna, J Chem Phys, 97, p 1990 (1992).

15.108 server command

15.108.1 Syntax

```
server protocol
```

- protocol = *md* or *mc*

15.108.2 Examples

```
server md
```

15.108.3 Description

This command starts LAMMPS running in "server" mode, where it receives messages from a separate "client" code and responds by sending a reply message back to the client. The specified *protocol* determines the format and content of messages LAMMPS expects to receive and how it responds.

The *Howto client/server* doc page gives an overview of client/server coupling of LAMMPS with another code where one code is the "client" and sends request messages to a "server" code. The server responds to each request with a reply message. This enables the two codes to work in tandem to perform a simulation.

When this command is invoked, LAMMPS will run in server mode in an endless loop, waiting for messages from the client code. The client signals when it is done sending messages to LAMMPS, at which point the loop will exit, and the remainder of the LAMMPS input script will be processed.

The *protocol* argument defines the format and content of messages that will be exchanged between the two codes. The current options are:

- *md* = run dynamics with another code
- *mc* = perform Monte Carlo moves with another code

For protocol *md*, LAMMPS can be either a client (via the *fix client/md* command) or server. See the *server md* doc page for details on the protocol.

For protocol *mc*, LAMMPS can be the server. See the *server mc* doc page for details on the protocol.

15.108.4 Restrictions

This command is part of the MESSAGE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

A script that uses this command must also use the *message* command to setup the messaging protocol with the other client code.

15.108.5 Related commands

message, *fix client/md*

Default: none

15.109 server mc command

15.109.1 Syntax

```
server mc
```

mc = the protocol argument to the *server* command

15.109.2 Examples

```
server mc
```

15.109.3 Description

This command starts LAMMPS running in "server" mode, where it will expect messages from a separate "client" code that match the *mc* protocol for format and content explained below. For each message LAMMPS receives it will send a message back to the client.

The *Howto client/server* doc page gives an overview of client/server coupling of LAMMPS with another code where one code is the "client" and sends request messages to a "server" code. The server responds to each request with a reply message. This enables the two codes to work in tandem to perform a simulation.

When this command is invoked, LAMMPS will run in server mode in an endless loop, waiting for messages from the client code. The client signals when it is done sending messages to LAMMPS, at which point the loop will exit, and the remainder of the LAMMPS script will be processed.

The *server* doc page gives other options for using LAMMPS See an example of how this command is used in examples/COUPLE/lammps_mc/in.server.

When using this command, LAMMPS (as the server code) receives instructions from a Monte Carlo (MC) driver to displace random atoms, compute the energy before and after displacement, and run dynamics to equilibrate the system.

The MC driver performs the random displacements on random atoms, accepts or rejects the move in an MC sense, and orchestrates the MD runs.

The format and content of the exchanged messages are explained here in a conceptual sense. Python-style pseudo code for the library calls to the CSlib is shown, which performs the actual message exchange between the two codes. See the CSlib website doc pages for more details on the actual library syntax. The "cs" object in this pseudo code is a pointer to an instance of the CSlib.

See the src/MESSAGE/server_mc.cpp file for details on how LAMMPS uses these messages. See the examples/COUPLE/lammps_mc/mc.cpp file for an example of how an MC driver code can use these messages.

Define NATOMS=1, EINIT=2, DISPLACE=3, ACCEPT=4, RUN=5.

Client sends one of these kinds of message:

```
cs->send(NATOMS,0)       # msgID = 1 with no fields

cs->send(EINIT,0)        # msgID = 2 with no fields

cs->send(DISPLACE,2)     # msgID = 3 with 2 fields
cs->pack_int(1,ID)         # 1st field = ID of atom to displace
cs->pack(2,3,xnew)       # 2nd field = new xyz coords of displaced atom

cs->send(ACCEPT,1)       # msgID = 4 with 1 field
cs->pack_int(1,flag)     # 1st field = accept/reject flag

cs->send(RUN,1)          # msgID = 5 with 1 field
cs->pack_int(1,nsteps)   # 1st field = # of timesteps to run MD
```

Server replies:

```
cs->send(NATOMS,1)       # msgID = 1 with 1 field
cs->pack_int(1,natoms)   # 1st field = number of atoms

cs->send(EINIT,2)          # msgID = 2 with 2 fields
cs->pack_double(1,poteng)  # 1st field = potential energy of system
cs->pack(2,3*natoms,x)     # 2nd field = 3N coords of Natoms

cs->send(DISPLACE,1)       # msgID = 3 with 1 field
cs->pack_double(1,poteng)  # 1st field = new potential energy of system

cs->send(ACCEPT,0)       # msgID = 4 with no fields

cs->send(RUN,0)          # msgID = 5 with no fields
```

15.109.4 Restrictions

This command is part of the MESSAGE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

A script that uses this command must also use the *message* command to setup the messaging protocol with the other client code.

15.109.5 Related commands

message

Default: none

15.110 server md command

15.110.1 Syntax

```
server md
```

md = the protocol argument to the *server* command

15.110.2 Examples

```
server md
```

15.110.3 Description

This command starts LAMMPS running in "server" mode, where it will expect messages from a separate "client" code that match the *md* protocol for format and content explained below. For each message LAMMPS receives it will send a message back to the client.

The *Howto client/server* doc page gives an overview of client/server coupling of LAMMPS with another code where one code is the "client" and sends request messages to a "server" code. The server responds to each request with a reply message. This enables the two codes to work in tandem to perform a simulation.

When this command is invoked, LAMMPS will run in server mode in an endless loop, waiting for messages from the client code. The client signals when it is done sending messages to LAMMPS, at which point the loop will exit, and the remainder of the LAMMPS script will be processed.

The *server* doc page gives other options for using LAMMPS in server mode. See an example of how this command is used in examples/message/in.message.server.

When using this command, LAMMPS (as the server code) receives the current coordinates of all particles from the client code each timestep, computes their interaction, and returns the energy, forces, and pressure for the interacting particles to the client code, so it can complete the timestep. This command could also be used with a client code that performs energy minimization, using the server to compute forces and energy each iteration of its minimizer.

When using the *fix client/md* command, LAMMPS (as the client code) does the timestepping and receives needed energy, forces, and pressure values from the server code.

The format and content of the exchanged messages are explained here in a conceptual sense. Python-style pseudo code for the library calls to the CSlib is shown, which performs the actual message exchange between the two codes. See the CSlib website doc pages for more details on the actual library syntax. The "cs" object in this pseudo code is a pointer to an instance of the CSlib.

See the src/MESSAGE/server_md.cpp and src/MESSAGE/fix_client_md.cpp files for details on how LAMMPS uses these messages. See the examples/COUPLE/lammps_vasp/vasp_wrap.py or examples/COUPLE/lammps_nwchem/nwchem_wrap.py files for examples of how a quantum code (VASP or NWChem) can use these messages.

The following pseudo-code uses these values, defined as enums.

Define:

```
SETUP=1, STEP=2
DIM=1, PERIODICITY=2, ORIGIN=3, BOX=4, NATOMS=5, NTYPES=6, TYPES=7, COORDS=8, UNITS-9,
↪ CHARGE=10
FORCES=1, ENERGY=2, PRESSURE=3, ERROR=4
```

Client sends 2 kinds of messages:

```
# required fields: DIM, PERIODICTY, ORIGIN, BOX, NATOMS, NTYPES, TYPES, COORDS
# optional fields: UNITS, CHARGE

cs->send(SETUP,nfields)        # msgID with nfields

cs->pack_int(DIM,dim)          # dimension (2,3) of simulation
cs->pack(PERIODICITY,3,xyz)    # periodicity flags in 3 dims
cs->pack(ORIGIN,3,origin)      # lower-left corner of simulation box
cs->pack(BOX,9,box)            # 3 edge vectors of simulation box
cs->pack_int(NATOMS,natoms)    # total number of atoms
cs->pack_int(NTYPES,ntypes)    # number of atom types
cs->pack(TYPES,natoms,type)    # vector of per-atom types
cs->pack(COORDS,3*natoms,x)    # vector of 3N atom coords
cs->pack_string(UNITS,units)   # units = "lj", "real", "metal", etc
cs->pack(CHARGE,natoms,q)      # vector of per-atom charge

# required fields: COORDS
# optional fields: ORIGIN, BOX

cs->send(STEP,nfields)         # msgID with nfields

cs->pack(COORDS,3*natoms,x)    # vector of 3N atom coords
cs->pack(ORIGIN,3,origin)      # lower-left corner of simulation box
cs->pack(BOX,9,box)            # 3 edge vectors of simulation box
```

Server replies to either kind of message:

```
# required fields: FORCES, ENERGY, PRESSURE
# optional fields: ERROR

cs->send(msgID,nfields)      # msgID with nfields
cs->pack(FORCES,3*Natoms,f)  # vector of 3N forces on atoms
cs->pack(ENERGY,1,poteng)    # total potential energy of system
cs->pack(PRESSURE,6,press)   # global pressure tensor (6-vector)
cs->pack_int(ERROR,flag)     # server had an error (e.g. DFT non-convergence)
```

The units for various quantities that are sent and received iva messages are defined for atomic-scale simulations in the table below. The client and server codes (including LAMMPS) can use internal units different than these (e.g. *real units* in LAMMPS), so long as they convert to these units for messaging.

- COORDS, ORIGIN, BOX = Angstroms
- CHARGE = multiple of electron charge (1.0 is a proton)
- ENERGY = eV
- FORCES = eV/Angstrom
- PRESSURE = bars

Note that these are *metal units* in LAMMPS.

If you wish to run LAMMPS in another its non-atomic units, e.g. *lj units*, then the client and server should exchange a UNITS message as indicated above, and both the client and server should agree on the units for the data they exchange.

15.110.4 Restrictions

This command is part of the MESSAGE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

15.110.5 Related commands

message, *fix client/md*

Default: none

15.111 set command

15.111.1 Syntax

```
set style ID keyword values ...
```

- style = *atom* or *type* or *mol* or *group* or *region*
- ID = atom ID range or type range or mol ID range or group ID or region ID
- one or more keyword/value pairs may be appended
- keyword = *type* or *type/fraction* or *type/ratio* or *type/subset* or *mol* or *x* or *y* or *z* or *charge* or *dipole* or *dipole/random* or *quat* or *spin* or *spin/random* or *quat* or *quat/random* or *diameter* or *shape* or *length* or *tri* or *theta* or *theta/random* or *angmom* or *omega* or *mass* or *density* or *density/disc* or *volume* or *image* or *bond* or *angle* or *dihedral* or *improper* or *meso/e* or *meso/cv* or *meso/rho* or *smd/contact/radius* or *smd/mass/density* or *dpd/theta* or *edpd/temp* or *edpd/cv* or *cc* or *i_name* or *d_name*

```
type value = atom type
  value can be an atom-style variable (see below)
type/fraction values = type fraction seed
  type = new atom type
  fraction = approximate fraction of selected atoms to set to new atom␣
↪type
  seed = random # seed (positive integer)
type/ratio values = type fraction seed
  type = new atom type
  fraction = exact fraction of selected atoms to set to new atom type
  seed = random # seed (positive integer)
type/subset values = type Nsubset seed
  type = new atom type
  Nsubset = exact number of selected atoms to set to new atom type
  seed = random # seed (positive integer)
mol value = molecule ID
  value can be an atom-style variable (see below)
```

```
x,y,z value = atom coordinate (distance units)
  value can be an atom-style variable (see below)
vx,vy,vz value = atom velocity (velocity units)
  value can be an atom-style variable (see below)
charge value = atomic charge (charge units)
  value can be an atom-style variable (see below)
dipole values = x y z
  x,y,z = orientation of dipole moment vector
  any of x,y,z can be an atom-style variable (see below)
dipole/random value = seed Dlen
  seed = random # seed (positive integer) for dipole moment orientations
  Dlen = magnitude of dipole moment (dipole units)
spin values = g x y z
  g = magnitude of magnetic spin vector (in Bohr magneton's unit)
  x,y,z = orientation of magnetic spin vector
  any of x,y,z can be an atom-style variable (see below)
spin/random value = seed Dlen
  seed = random # seed (positive integer) for magnetic spin orientations
  Dlen = magnitude of magnetic spin vector (in Bohr magneton's unit)
quat values = a b c theta
  a,b,c = unit vector to rotate particle around via right-hand rule
  theta = rotation angle (degrees)
  any of a,b,c,theta can be an atom-style variable (see below)
quat/random value = seed
  seed = random # seed (positive integer) for quaternion orientations
diameter value = diameter of spherical particle (distance units)
  value can be an atom-style variable (see below)
shape value = Sx Sy Sz
  Sx,Sy,Sz = 3 diameters of ellipsoid (distance units)
length value = len
  len = length of line segment (distance units)
  len can be an atom-style variable (see below)
tri value = side
  side = side length of equilateral triangle (distance units)
  side can be an atom-style variable (see below)
theta value = angle (degrees)
  angle = orientation of line segment with respect to x-axis
  angle can be an atom-style variable (see below)
theta/random value = seed
  seed = random # seed (positive integer) for line segment orienations
angmom values = Lx Ly Lz
  Lx,Ly,Lz = components of angular momentum vector (distance-mass-velocity␣
↪units)
  any of Lx,Ly,Lz can be an atom-style variable (see below)
omega values = Wx Wy Wz
  Wx,Wy,Wz = components of angular velocity vector (radians/time units)
  any of wx,wy,wz can be an atom-style variable (see below)
mass value = per-atom mass (mass units)
  value can be an atom-style variable (see below)
density value = particle density for a sphere or ellipsoid (mass/
↪distance^3 units), or for a triangle (mass/distance^2 units) or line␣
↪(mass/distance units) particle
  value can be an atom-style variable (see below)
density/disc value = particle density for a 2d disc or ellipse (mass/
```

```
↪distance^2 units)
  value can be an atom-style variable (see below)
volume value = particle volume for Peridynamic particle (distance^3 units)
  value can be an atom-style variable (see below)
image nx ny nz
  nx,ny,nz = which periodic image of the simulation box the atom is in
  any of nx,ny,nz can be an atom-style variable (see below)
bond value = bond type for all bonds between selected atoms
angle value = angle type for all angles between selected atoms
dihedral value = dihedral type for all dihedrals between selected atoms
improper value = improper type for all impropers between selected atoms
meso/e value = energy of SPH particles (need units)
  value can be an atom-style variable (see below)
meso/cv value = heat capacity of SPH particles (need units)
  value can be an atom-style variable (see below)
meso/rho value = density of SPH particles (need units)
  value can be an atom-style variable (see below)
smd/contact/radius = radius for short range interactions, i.e. contact␣
↪and friction
  value can be an atom-style variable (see below)
smd/mass/density = set particle mass based on volume by providing a mass␣
↪density
  value can be an atom-style variable (see below)
dpd/theta value = internal temperature of DPD particles (temperature␣
↪units)
  value can be an atom-style variable (see below)
  value can be NULL which sets internal temp of each particle to KE temp
edpd/temp value = temperature of eDPD particles (temperature units)
  value can be an atom-style variable (see below)
edpd/cv value = volumetric heat capacity of eDPD particles (energy/
↪temperature/volume units)
  value can be an atom-style variable (see below)
cc values = index cc
  index = index of a chemical species (1 to Nspecies)
  cc = chemical concentration of tDPD particles for a species (mole/
↪volume units)
i_name value = value for custom integer vector with name
d_name value = value for custom floating-point vector with name
```

15.111.2 Examples

```
set group solvent type 2
set group solvent type/fraction 2 0.5 12393
set group edge bond 4
set region half charge 0.5
set type 3 charge 0.5
set type 1*3 charge 0.5
set atom * charge v_atomfile
set atom 100*200 x 0.5 y 1.0
set atom 100 vx 0.0 vy 0.0 vz -1.0
set atom 1492 type 3
```

15.111.3 Description

Set one or more properties of one or more atoms. Since atom properties are initially assigned by the *read_data*, *read_restart* or *create_atoms* commands, this command changes those assignments. This can be useful for overriding the default values assigned by the *create_atoms* command (e.g. charge = 0.0). It can be useful for altering pairwise and molecular force interactions, since force-field coefficients are defined in terms of types. It can be used to change the labeling of atoms by atom type or molecule ID when they are output in *dump* files. It can also be useful for debugging purposes; i.e. positioning an atom at a precise location to compute subsequent forces or energy.

Note that the *style* and *ID* arguments determine which atoms have their properties reset. The remaining keywords specify which properties to reset and what the new values are. Some strings like *type* or *mol* can be used as a style and/or a keyword.

This section describes how to select which atoms to change the properties of, via the *style* and *ID* arguments.

The style *atom* selects all the atoms in a range of atom IDs. The style *type* selects all the atoms in a range of types. The style *mol* selects all the atoms in a range of molecule IDs.

In each of the range cases, the range can be specified as a single numeric value, or a wildcard asterisk can be used to specify a range of values. This takes the form "*" or "*n" or "n*" or "m*n". For example, for the style *type*, if N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). For all the styles except *mol*, the lowest value for the wildcard is 1; for *mol* it is 0.

The style *group* selects all the atoms in the specified group. The style *region* selects all the atoms in the specified geometric region. See the *group* and *region* commands for details of how to specify a group or region.

This section describes the keyword options for which properties to change, for the selected atoms.

Note that except where explicitly prohibited below, all of the keywords allow an *atom-style or atomfile-style variable* to be used as the specified value(s). If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated, and its resulting per-atom value used to determine the value assigned to each selected atom. Note that the per-atom value from the variable will be ignored for atoms that are not selected via the *style* and *ID* settings explained above. A simple way to use per-atom values from the variable to reset a property for all atoms is to use style *atom* with *ID* = "*"; this selects all atom IDs.

Atom-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. They can also include per-atom values, such as atom coordinates. Thus it is easy to specify a time-dependent or spatially-dependent set of per-atom values. As explained on the *variable* doc page, atomfile-style variables can be used in place of atom-style variables, and thus as arguments to the set command. Atomfile-style variables read their per-atoms values from a file.

Note: Atom-style and atomfile-style variables return floating point per-atom values. If the values are assigned to an integer variable, such as the molecule ID, then the floating point value is truncated to its integer portion, e.g. a value of 2.6 would become 2.

Keyword *type* sets the atom type for all selected atoms. The specified value must be from 1 to ntypes, where ntypes was set by the *create_box* command or the *atom types* field in the header of the data file read by the *read_data* command.

Keyword *type/fraction* sets the atom type for a fraction of the selected atoms. The actual number of atoms changed is not guaranteed to be exactly the specified fraction (0 <= *fraction* <= 1), but should be statistically close. Random numbers are used in such a way that a particular atom is changed or not changed, regardless of how many processors are being used. This keyword does not allow use of an atom-style variable.

Keywords *type/ratio* and *type/subset* also set the atom type for a fraction of the selected atoms. The actual number of atoms changed will be exactly the requested number. For *type/ratio* the specified fraction (0 <= *fraction* <= 1) determines the number. For *type/subset*, the specified *Nsubset* is the number. An iterative algorithm is used which insures the correct number of atoms are selected, in a perfectly random fashion. Which atoms are selected will change with the number of processors used. These keywords do not allow use of an atom-style variable.

Keyword *mol* sets the molecule ID for all selected atoms. The *atom style* being used must support the use of molecule IDs.

Keywords *x*, *y*, *z*, and *charge* set the coordinates or charge of all selected atoms. For *charge*, the *atom style* being used must support the use of atomic charge. Keywords *vx*, *vy*, and *vz* set the velocities of all selected atoms.

Keyword *dipole* uses the specified x,y,z values as components of a vector to set as the orientation of the dipole moment vectors of the selected atoms. The magnitude of the dipole moment is set by the length of this orientation vector.

Keyword *dipole/random* randomizes the orientation of the dipole moment vectors for the selected atoms and sets the magnitude of each to the specified *Dlen* value. For 2d systems, the z component of the orientation is set to 0.0. Random numbers are used in such a way that the orientation of a particular atom is the same, regardless of how many processors are being used. This keyword does not allow use of an atom-style variable.

Keyword *spin* uses the specified g value to set the magnitude of the magnetic spin vectors, and the x,y,z values as components of a vector to set as the orientation of the magnetic spin vectors of the selected atoms.

Keyword *spin/random* randomizes the orientation of the magnetic spin vectors for the selected atoms and sets the magnitude of each to the specified *Dlen* value.

Keyword *quat* uses the specified values to create a quaternion (4-vector) that represents the orientation of the selected atoms. The particles must define a quaternion for their orientation (e.g. ellipsoids, triangles, body particles) as defined by the *atom_style* command. Note that particles defined by *atom_style ellipsoid* have 3 shape parameters. The 3 values must be non-zero for each particle set by this command. They are used to specify the aspect ratios of an ellipsoidal particle, which is oriented by default with its x-axis along the simulation box's x-axis, and similarly for y and z. If this body is rotated (via the right-hand rule) by an angle theta around a unit rotation vector (a,b,c), then the quaternion that represents its new orientation is given by (cos(theta/2), a*sin(theta/2), b*sin(theta/2), c*sin(theta/2)). The theta and a,b,c values are the arguments to the *quat* keyword. LAMMPS normalizes the quaternion in case (a,b,c) was not specified as a unit vector. For 2d systems, the a,b,c values are ignored, since a rotation vector of (0,0,1) is the only valid choice.

Keyword *quat/random* randomizes the orientation of the quaternion for the selected atoms. The particles must define a quaternion for their orientation (e.g. ellipsoids, triangles, body particles) as defined by the *atom_style* command. Random numbers are used in such a way that the orientation of a particular atom is the same, regardless of how many processors are being used. For 2d systems, only orientations in the xy plane are generated. As with keyword *quat*, for ellipsoidal particles, the 3 shape values must be non-zero for each particle set by this command. This keyword does not allow use of an atom-style variable.

Keyword *diameter* sets the size of the selected atoms. The particles must be finite-size spheres as defined by the *atom_style sphere* command. The diameter of a particle can be set to 0.0, which means they will be treated as point particles. Note that this command does not adjust the particle mass, even if it was defined with a density, e.g. via the *read_data* command.

Keyword *shape* sets the size and shape of the selected atoms. The particles must be ellipsoids as defined by the *atom_style ellipsoid* command. The *Sx*, *Sy*, *Sz* settings are the 3 diameters of the ellipsoid in each direction. All 3 can be set to the same value, which means the ellipsoid is effectively a sphere. They can also all be set to 0.0 which means the particle will be treated as a point particle. Note that this command does not adjust the particle mass, even if it was defined with a density, e.g. via the *read_data* command.

Keyword *length* sets the length of selected atoms. The particles must be line segments as defined by the *atom_style line* command. If the specified value is non-zero the line segment is (re)set to a length = the specified value, centered around the particle position, with an orientation along the x-axis. If the specified value is 0.0, the particle will become

a point particle. Note that this command does not adjust the particle mass, even if it was defined with a density, e.g. via the *read_data* command.

Keyword *tri* sets the size of selected atoms. The particles must be triangles as defined by the *atom_style tri* command. If the specified value is non-zero the triangle is (re)set to be an equilateral triangle in the xy plane with side length = the specified value, with a centroid at the particle position, with its base parallel to the x axis, and the y-axis running from the center of the base to the top point of the triangle. If the specified value is 0.0, the particle will become a point particle. Note that this command does not adjust the particle mass, even if it was defined with a density, e.g. via the *read_data* command.

Keyword *theta* sets the orientation of selected atoms. The particles must be line segments as defined by the *atom_style line* command. The specified value is used to set the orientation angle of the line segments with respect to the x axis.

Keyword *theta/random* randomizes the orientation of theta for the selected atoms. The particles must be line segments as defined by the *atom_style line* command. Random numbers are used in such a way that the orientation of a particular atom is the same, regardless of how many processors are being used. This keyword does not allow use of an atom-style variable.

Keyword *angmom* sets the angular momentum of selected atoms. The particles must be ellipsoids as defined by the *atom_style ellipsoid* command or triangles as defined by the *atom_style tri* command. The angular momentum vector of the particles is set to the 3 specified components.

Keyword *omega* sets the angular velocity of selected atoms. The particles must be spheres as defined by the *atom_style sphere* command. The angular velocity vector of the particles is set to the 3 specified components.

Keyword *mass* sets the mass of all selected particles. The particles must have a per-atom mass attribute, as defined by the *atom_style* command. See the "mass" command for how to set mass values on a per-type basis.

Keyword *density* or *density/disc* also sets the mass of all selected particles, but in a different way. The particles must have a per-atom mass attribute, as defined by the *atom_style* command. If the atom has a radius attribute (see *atom_style sphere*) and its radius is non-zero, its mass is set from the density and particle volume for 3d systems (the input density is assumed to be in mass/distance^3 units). For 2d, the default is for LAMMPS to model particles with a radius attribute as spheres. However, if the *density/disc* keyword is used, then they can be modeled as 2d discs (circles). Their mass is set from the density and particle area (the input density is assumed to be in mass/distance^2 units).

If the atom has a shape attribute (see *atom_style ellipsoid*) and its 3 shape parameters are non-zero, then its mass is set from the density and particle volume (the input density is assumed to be in mass/distance^3 units). The *density/disc* keyword has no effect; it does not (yet) treat 3d ellipsoids as 2d ellipses.

If the atom has a length attribute (see *atom_style line*) and its length is non-zero, then its mass is set from the density and line segment length (the input density is assumed to be in mass/distance units). If the atom has an area attribute (see *atom_style tri*) and its area is non-zero, then its mass is set from the density and triangle area (the input density is assumed to be in mass/distance^2 units).

If none of these cases are valid, then the mass is set to the density value directly (the input density is assumed to be in mass units).

Keyword *volume* sets the volume of all selected particles. Currently, only the *atom_style peri* command defines particles with a volume attribute. Note that this command does not adjust the particle mass.

Keyword *image* sets which image of the simulation box the atom is considered to be in. An image of 0 means it is inside the box as defined. A value of 2 means add 2 box lengths to get the true value. A value of -1 means subtract 1 box length to get the true value. LAMMPS updates these flags as atoms cross periodic boundaries during the simulation. The flags can be output with atom snapshots via the *dump* command. If a value of NULL is specified for any of nx,ny,nz, then the current image value for that dimension is unchanged. For non-periodic dimensions only a value of 0 can be specified. This command can be useful after a system has been equilibrated and atoms have diffused one or more box lengths in various directions. This command can then reset the image values for atoms so that they are effectively inside the simulation box, e.g if a diffusion coefficient is about to be measured via the *compute msd* command. Care should be taken not to reset the image flags of two atoms in a bond to the same value if the

bond straddles a periodic boundary (rather they should be different by +/- 1). This will not affect the dynamics of a simulation, but may mess up analysis of the trajectories if a LAMMPS diagnostic or your own analysis relies on the image flags to unwrap a molecule which straddles the periodic box.

Keywords *bond*, *angle*, *dihedral*, and *improper*, set the bond type (angle type, etc) of all bonds (angles, etc) of selected atoms to the specified value from 1 to nbondtypes (nangletypes, etc). All atoms in a particular bond (angle, etc) must be selected atoms in order for the change to be made. The value of nbondtype (nangletypes, etc) was set by the *bond types* (*angle types*, etc) field in the header of the data file read by the *read_data* command. These keywords do not allow use of an atom-style variable.

Keywords *meso/e*, *meso/cv*, and *meso/rho* set the energy, heat capacity, and density of smoothed particle hydrodynamics (SPH) particles. See this PDF guide to using SPH in LAMMPS.

Keyword *smd/mass/density* sets the mass of all selected particles, but it is only applicable to the Smooth Mach Dynamics package USER-SMD. It assumes that the particle volume has already been correctly set and calculates particle mass from the provided mass density value.

Keyword *smd/contact/radius* only applies to simulations with the Smooth Mach Dynamics package USER-SMD. Itsets an interaction radius for computing short-range interactions, e.g. repulsive forces to prevent different individual physical bodies from penetrating each other. Note that the SPH smoothing kernel diameter used for computing long range, nonlocal interactions, is set using the *diameter* keyword.

Keyword *dpd/theta* sets the internal temperature of a DPD particle as defined by the USER-DPD package. If the specified value is a number it must be >= 0.0. If the specified value is NULL, then the kinetic temperature Tkin of each particle is computed as 3/2 k Tkin = KE = 1/2 m v^2 = 1/2 m (vx*vx+vy*vy+vz*vz). Each particle's internal temperature is set to Tkin. If the specified value is an atom-style variable, then the variable is evaluated for each particle. If a value >= 0.0, the internal temperature is set to that value. If it is < 0.0, the computation of Tkin is performed and the internal temperature is set to that value.

Keywords *edpd/temp* and *edpd/cv* set the temperature and volumetric heat capacity of an eDPD particle as defined by the USER-MESO package. Currently, only *atom_style edpd* defines particles with these attributes. The values for the temperature and heat capacity must be positive.

Keyword *cc* sets the chemical concentration of a tDPD particle for a specified species as defined by the USER-MESO package. Currently, only *atom_style tdpd* defines particles with this attribute. An integer for "index" selects a chemical species (1 to Nspecies) where Nspecies is set by the atom_style command. The value for the chemical concentration must be >= 0.0.

Keywords *i_name* and *d_name* refer to custom integer and floating-point properties that have been added to each atom via the *fix property/atom* command. When that command is used specific names are given to each attribute which are what is specified as the "name" portion of *i_name* or *d_name*.

15.111.4 Restrictions

You cannot set an atom attribute (e.g. *mol* or *q* or *volume*) if the *atom_style* does not have that attribute.

This command requires inter-processor communication to coordinate the setting of bond types (angle types, etc). This means that your system must be ready to perform a simulation before using one of these keywords (force fields set, atom mass set, etc). This is not necessary for other keywords.

Using the *region* style with the bond (angle, etc) keywords can give unpredictable results if there are bonds (angles, etc) that straddle periodic boundaries. This is because the region may only extend up to the boundary and partner atoms in the bond (angle, etc) may have coordinates outside the simulation box if they are ghost atoms.

15.111.5 Related commands

create_box, *create_atoms*, *read_data*

Default: none

15.112 shell command

15.112.1 Syntax

```
shell cmd args
```

- cmd = *cd* or *mkdir* or *mv* or *rm* or *rmdir* or *putenv* or arbitrary command

```
cd arg = dir
  dir = directory to change to
mkdir args = dir1 dir2 ...
  dir1,dir2 = one or more directories to create
mv args = old new
  old = old filename
  new = new filename
rm args = file1 file2 ...
  file1,file2 = one or more filenames to delete
rmdir args = dir1 dir2 ...
  dir1,dir2 = one or more directories to delete
putenv args = var1=value1 var2=value2
  var=value = one of more definitions of environment variables
anything else is passed as a command to the shell for direct execution
```

15.112.2 Examples

```
shell cd sub1
shell cd ..
shell mkdir tmp1 tmp2 tmp3
shell rmdir tmp1
shell mv log.lammps hold/log.1
shell rm TMP/file1 TMP/file2
shell putenv LAMMPS_POTENTIALS=../../potentials
shell my_setup file1 10 file2
shell my_post_process 100 dump.out
```

15.112.3 Description

Execute a shell command. A few simple file-based shell commands are supported directly, in Unix-style syntax. Any command not listed above is passed as-is to the C-library system() call, which invokes the command in a shell.

This is means to invoke other commands from your input script. For example, you can move files around in preparation for the next section of the input script. Or you can run a program that pre-processes data for input into LAMMPS. Or you can run a program that post-processes LAMMPS output data.

With the exception of *cd*, all commands, including ones invoked via a system() call, are executed by only a single processor, so that files/directories are not being manipulated by multiple processors.

The *cd* cmd executes the Unix "cd" command to change the working directory. All subsequent LAMMPS commands that read/write files will use the new directory. All processors execute this command.

The *mkdir* cmd executes the Unix "mkdir" command to create one or more directories.

The *mv* cmd executes the Unix "mv" command to rename a file and/or move it to a new directory.

The *rm* cmd executes the Unix "rm" command to remove one or more files.

The *rmdir* cmd executes the Unix "rmdir" command to remove one or more directories. A directory must be empty to be successfully removed.

The *putenv* cmd defines or updates an environment variable directly. Since this command does not pass through the shell, no shell variable expansion or globbing is performed, only the usual substitution for LAMMPS variables defined with the *variable* command is performed. The resulting string is then used literally.

Any other cmd is passed as-is to the shell along with its arguments as one string, invoked by the C-library system() call. For example, these lines in your input script:

```
variable n equal 10
variable foo string file2
shell my_setup file1 $n ${foo}
```

would be the same as invoking

```
% my_setup file1 10 file2
```

from a command-line prompt. The executable program "my_setup" is run with 3 arguments: file1 10 file2.

15.112.4 Restrictions

LAMMPS does not detect errors or print warnings when any of these commands execute. E.g. if the specified directory does not exist, executing the *cd* command will silently do nothing.

Related commands: none

Default: none

15.113 special_bonds command

15.113.1 Syntax

```
special_bonds keyword values ...
```

- one or more keyword/value pairs may be appended
- keyword = *amber* or *charmm* or *dreiding* or *fene* or *lj/coul* or *lj* or *coul* or *angle* or *dihedral*

```
amber values = none
charmm values = none
dreiding values = none
fene values = none
lj/coul values = w1,w2,w3
  w1,w2,w3 = weights (0.0 to 1.0) on pairwise Lennard-Jones and Coulombic␣
↪interactions
lj values = w1,w2,w3
  w1,w2,w3 = weights (0.0 to 1.0) on pairwise Lennard-Jones interactions
```

```
coul values = w1,w2,w3
  w1,w2,w3 = weights (0.0 to 1.0) on pairwise Coulombic interactions
angle value = yes or no
dihedral value = yes or no
```

Examples:

```
special_bonds amber
special_bonds charmm
special_bonds fene dihedral no
special_bonds lj/coul 0.0 0.0 0.5 angle yes dihedral yes
special_bonds lj 0.0 0.0 0.5 coul 0.0 0.0 0.0 dihedral yes
```

15.113.2 Description

Set weighting coefficients for pairwise energy and force contributions between pairs of atoms that are also permanently bonded to each other, either directly or via one or two intermediate bonds. These weighting factors are used by nearly all *pair styles* in LAMMPS that compute simple pairwise interactions. Permanent bonds between atoms are specified by defining the bond topology in the data file read by the *read_data* command. Typically a *bond_style* command is also used to define a bond potential. The rationale for using these weighting factors is that the interaction between a pair of bonded atoms is all (or mostly) specified by the bond, angle, dihedral potentials, and thus the non-bonded Lennard-Jones or Coulombic interaction between the pair of atoms should be excluded (or reduced by a weighting factor).

Note: These weighting factors are NOT used by *pair styles* that compute many-body interactions, since the "bonds" that result from such interactions are not permanent, but are created and broken dynamically as atom conformations change. Examples of pair styles in this category are EAM, MEAM, Stillinger-Weber, Tersoff, COMB, AIREBO, and ReaxFF. In fact, it generally makes no sense to define permanent bonds between atoms that interact via these potentials, though such bonds may exist elsewhere in your system, e.g. when using the *pair_style hybrid* command. Thus LAMMPS ignores special_bonds settings when many-body potentials are calculated. Please note, that the existence of explicit bonds for atoms that are described by a many-body potential will alter the neighbor list and thus can render the computation of those interactions invalid, since those pairs are not only used to determine direct pairwise interactions but also neighbors of neighbors and more. The recommended course of action is to remove such bonds, or - if that is not possible - use a special bonds setting of 1.0 1.0 1.0.

Note: Unlike some commands in LAMMPS, you cannot use this command multiple times in an incremental fashion: e.g. to first set the LJ settings and then the Coulombic ones. Each time you use this command it sets all the coefficients to default values and only overrides the one you specify, so you should set all the options you need each time you use it. See more details at the bottom of this page.

The Coulomb factors are applied to any Coulomb (charge interaction) term that the potential calculates. The LJ factors are applied to the remaining terms that the potential calculates, whether they represent LJ interactions or not. The weighting factors are a scaling pre-factor on the energy and force between the pair of atoms. A value of 1.0 means include the full interaction; a value of 0.0 means exclude it completely.

The 1st of the 3 coefficients (LJ or Coulombic) is the weighting factor on 1-2 atom pairs, which are pairs of atoms directly bonded to each other. The 2nd coefficient is the weighting factor on 1-3 atom pairs which are those separated by 2 bonds (e.g. the two H atoms in a water molecule). The 3rd coefficient is the weighting factor on 1-4 atom pairs which are those separated by 3 bonds (e.g. the 1st and 4th atoms in a dihedral interaction). Thus if the 1-2 coefficient is set to 0.0, then the pairwise interaction is effectively turned off for all pairs of atoms bonded to each other. If it is set to 1.0, then that interaction will be at full strength.

Note: For purposes of computing weighted pairwise interactions, 1-3 and 1-4 interactions are not defined from the list of angles or dihedrals used by the simulation. Rather, they are inferred topologically from the set of bonds specified when the simulation is defined from a data or restart file (see *read_data* or *read_restart* commands). Thus the set of 1-2,1-3,1-4 interactions that the weights apply to is the same whether angle and dihedral potentials are computed or not, and remains the same even if bonds are constrained, or turned off, or removed during a simulation.

The two exceptions to this rule are (a) if the *angle* or *dihedral* keywords are set to *yes* (see below), or (b) if the *delete_bonds* command is used with the *special* option that re-computes the 1-2,1-3,1-4 topologies after bonds are deleted; see the *delete_bonds* command for more details.

The *amber* keyword sets the 3 coefficients to 0.0, 0.0, 0.5 for LJ interactions and to 0.0, 0.0, 0.8333 for Coulombic interactions, which is the default for a commonly used version of the AMBER force field, where the last value is really 5/6. See *(Cornell)* for a description of the AMBER force field.

The *charmm* keyword sets the 3 coefficients to 0.0, 0.0, 0.0 for both LJ and Coulombic interactions, which is the default for a commonly used version of the CHARMM force field. Note that in pair styles *lj/charmm/coul/charmm* and *lj/charmm/coul/long* the 1-4 coefficients are defined explicitly, and these pairwise contributions are computed as part of the charmm dihedral style - see the *pair_coeff* and *dihedral_style* commands for more information. See *(MacKerell)* for a description of the CHARMM force field.

The *dreiding* keyword sets the 3 coefficients to 0.0, 0.0, 1.0 for both LJ and Coulombic interactions, which is the default for the Dreiding force field, as discussed in *(Mayo)*.

The *fene* keyword sets the 3 coefficients to 0.0, 1.0, 1.0 for both LJ and Coulombic interactions, which is consistent with a coarse-grained polymer model with *FENE bonds*. See *(Kremer)* for a description of FENE bonds.

The *lj/coul*, *lj*, and *coul* keywords allow the 3 coefficients to be set explicitly. The *lj/coul* keyword sets both the LJ and Coulombic coefficients to the same 3 values. The *lj* and *coul* keywords only set either the LJ or Coulombic coefficients. Use both of them if you wish to set the LJ coefficients to different values than the Coulombic coefficients.

The *angle* keyword allows the 1-3 weighting factor to be ignored for individual atom pairs if they are not listed as the first and last atoms in any angle defined in the simulation or as 1,3 or 2,4 atoms in any dihedral defined in the simulation. For example, imagine the 1-3 weighting factor is set to 0.5 and you have a linear molecule with 4 atoms and bonds as follows: 1-2-3-4. If your data file defines 1-2-3 as an angle, but does not define 2-3-4 as an angle or 1-2-3-4 as a dihedral, then the pairwise interaction between atoms 1 and 3 will always be weighted by 0.5, but different force fields use different rules for weighting the pairwise interaction between atoms 2 and 4. If the *angle* keyword is specified as *yes*, then the pairwise interaction between atoms 2 and 4 will be unaffected (full weighting of 1.0). If the *angle* keyword is specified as *no* which is the default, then the 2,4 interaction will also be weighted by 0.5.

The *dihedral* keyword allows the 1-4 weighting factor to be ignored for individual atom pairs if they are not listed as the first and last atoms in any dihedral defined in the simulation. For example, imagine the 1-4 weighting factor is set to 0.5 and you have a linear molecule with 5 atoms and bonds as follows: 1-2-3-4-5. If your data file defines 1-2-3-4 as a dihedral, but does not define 2-3-4-5 as a dihedral, then the pairwise interaction between atoms 1 and 4 will always be weighted by 0.5, but different force fields use different rules for weighting the pairwise interaction between atoms 2 and 5. If the *dihedral* keyword is specified as *yes*, then the pairwise interaction between atoms 2 and 5 will be unaffected (full weighting of 1.0). If the *dihedral* keyword is specified as *no* which is the default, then the 2,5 interaction will also be weighted by 0.5.

Note: LAMMPS stores and maintains a data structure with a list of the 1st, 2nd, and 3rd neighbors of each atom (within the bond topology of the system). If new bonds are created (or molecules added containing atoms with more special neighbors), the size of this list needs to grow. Note that adding a single bond always adds a new 1st neighbor but may also induce *many* new 2nd and 3rd neighbors, depending on the molecular topology of your system. Using the *extra/special/per/atom* keyword to either *read_data* or *create_box* reserves empty space in the list for this N additional

1st, 2nd, or 3rd neighbors to be added. If you do not do this, you may get an error when bonds (or molecules) are added.

Note: If you reuse this command in an input script, you should set all the options you need each time. This command cannot be used a 2nd time incrementally. E.g. these two commands:

```
special_bonds lj 0.0 1.0 1.0
special_bonds coul 0.0 0.0 1.0
```

are not the same as

```
special_bonds lj 0.0 1.0 1.0 coul 0.0 0.0 1.0
```

In the first case you end up with (after the 2nd command):

```
LJ: 0.0 0.0 0.0
Coul: 0.0 0.0 1.0
```

while only in the second case, you get the desired settings of:

```
LJ: 0.0 1.0 1.0
Coul: 0.0 0.0 1.0
```

This happens because the LJ (and Coul) settings are reset to their default values before modifying them, each time the *special_bonds* command is issued.

15.113.3 Restrictions

none

15.113.4 Related commands

delete_bonds, *fix bond/create*

15.113.5 Default

All 3 Lennard-Jones and 3 Coulombic weighting coefficients = 0.0, angle = no, dihedral = no.

(Cornell) Cornell, Cieplak, Bayly, Gould, Merz, Ferguson, Spellmeyer, Fox, Caldwell, Kollman, JACS 117, 5179-5197 (1995).

(Kremer) Kremer, Grest, J Chem Phys, 92, 5057 (1990).

(MacKerell) MacKerell, Bashford, Bellott, Dunbrack, Evanseck, Field, Fischer, Gao, Guo, Ha, et al, J Phys Chem, 102, 3586 (1998).

(Mayo) Mayo, Olfason, Goddard III, J Phys Chem, 94, 8897-8909 (1990).

15.114 suffix command

15.114.1 Syntax

```
suffix style args
```

- style = *off* or *on* or *gpu* or *intel* or *kk* or *omp* or *opt* or *hybrid*
- args = for hybrid style, default suffix to be used and alternative suffix

15.114.2 Examples

```
suffix off
suffix on
suffix gpu
suffix intel
suffix hybrid intel omp
suffix kk
```

15.114.3 Description

This command allows you to use variants of various styles if they exist. In that respect it operates the same as the *-suffix command-line switch*. It also has options to turn off or back on any suffix setting made via the command line.

The specified style can be *gpu*, *intel*, *kk*, *omp*, *opt* or *hybrid*. These refer to optional packages that LAMMPS can be built with, as described on the *Build package* doc page. The "gpu" style corresponds to the GPU package, the "intel" style to the USER-INTEL package, the "kk" style to the KOKKOS package, the "omp" style to the USER-OMP package, and the "opt" style to the OPT package.

These are the variants these packages provide:

- GPU = a handful of pair styles and the PPPM kspace_style, optimized to run on one or more GPUs or multicore CPU/GPU nodes
- USER-INTEL = a collection of pair styles and neighbor routines optimized to run in single, mixed, or double precision on CPUs and Intel(R) Xeon Phi(TM) co-processors.
- KOKKOS = a collection of atom, pair, and fix styles optimized to run using the Kokkos library on various kinds of hardware, including GPUs via CUDA and many-core chips via OpenMP or threading.
- USER-OMP = a collection of pair, bond, angle, dihedral, improper, kspace, compute, and fix styles with support for OpenMP multi-threading
- OPT = a handful of pair styles, cache-optimized for faster CPU performance
- HYBRID = a combination of two packages can be specified (see below)

As an example, all of the packages provide a *pair_style lj/cut* variant, with style names lj/cut/opt, lj/cut/omp, lj/cut/gpu, lj/cut/intel, or lj/cut/kk. A variant styles can be specified explicitly in your input script, e.g. pair_style lj/cut/gpu. If the suffix command is used with the appropriate style, you do not need to modify your input script. The specified suffix (opt,omp,gpu,intel,kk) is automatically appended whenever your input script command creates a new *atom*, *pair*, *bond*, *angle*, *dihedral*, *improper*, *kspace*, *fix*, *compute*, or *run* style. If the variant version does not exist, the standard version is created.

For "hybrid", two packages are specified. The first is used whenever available. If a style with the first suffix is not available, the style with the suffix for the second package will be used if available. For example, "hybrid intel omp"

will use styles from the USER-INTEL package as a first choice and styles from the USER-OMP package as a second choice if no USER-INTEL variant is available.

If the specified style is *off*, then any previously specified suffix is temporarily disabled, whether it was specified by a command-line switch or a previous suffix command. If the specified style is *on*, a disabled suffix is turned back on. The use of these 2 commands lets your input script use a standard LAMMPS style (i.e. a non-accelerated variant), which can be useful for testing or benchmarking purposes. Of course this is also possible by not using any suffix commands, and explicitly appending or not appending the suffix to the relevant commands in your input script.

Note: The default *run_style* verlet is invoked prior to reading the input script and is therefore not affected by a suffix command in the input script. The KOKKOS package requires "run_style verlet/kk", so when using the KOKKOS package it is necessary to either use the command line "-sf kk" command or add an explicit "run_style verlet" command to the input script.

15.114.4 Restrictions

none

15.114.5 Related commands

-suffix command-line switch

Default: none

15.115 tad command

15.115.1 Syntax

```
tad N t_event T_lo T_hi delta tmax compute-ID keyword value ...
```

- N = # of timesteps to run (not including dephasing/quenching)
- t_event = timestep interval between event checks
- T_lo = temperature at which event times are desired
- T_hi = temperature at which MD simulation is performed
- delta = desired confidence level for stopping criterion
- tmax = reciprocal of lowest expected pre-exponential factor (time units)
- compute-ID = ID of the compute used for event detection
- zero or more keyword/value pairs may be appended
- keyword = *min* or *neb* or *min_style* or *neb_style* or *neb_log*

```
min values = etol ftol maxiter maxeval
  etol = stopping tolerance for energy (energy units)
  ftol = stopping tolerance for force (force units)
  maxiter = max iterations of minimize
  maxeval = max number of force/energy evaluations
neb values = ftol N1 N2 Nevery
```

```
    etol = stopping tolerance for energy (energy units)
    ftol = stopping tolerance for force (force units)
    N1 = max # of iterations (timesteps) to run initial NEB
    N2 = max # of iterations (timesteps) to run barrier-climbing NEB
    Nevery = print NEB statistics every this many timesteps
  neb_style value = quickmin or fire
  neb_step value = dtneb
    dtneb = timestep for NEB damped dynamics minimization
  neb_log value = file where NEB statistics are printed
```

15.115.2 Examples

```
tad 2000 50 1800 2300 0.01 0.01 event
tad 2000 50 1800 2300 0.01 0.01 event &
    min 1e-05 1e-05 100 100 &
    neb 0.0 0.01 200 200 20 &
    min_style cg &
    neb_style fire &
    neb_log log.neb
```

15.115.3 Description

Run a temperature accelerated dynamics (TAD) simulation. This method requires two or more partitions to perform NEB transition state searches.

TAD is described in *this paper* by Art Voter. It is a method that uses accelerated dynamics at an elevated temperature to generate results at a specified lower temperature. A good overview of accelerated dynamics methods for such systems is given in *this review paper* from the same group. In general, these methods assume that the long-time dynamics is dominated by infrequent events i.e. the system is confined to low energy basins for long periods, punctuated by brief, randomly-occurring transitions to adjacent basins. TAD is suitable for infrequent-event systems, where in addition, the transition kinetics are well-approximated by harmonic transition state theory (hTST). In hTST, the temperature dependence of transition rates follows the Arrhenius relation. As a consequence a set of event times generated in a high-temperature simulation can be mapped to a set of much longer estimated times in the low-temperature system. However, because this mapping involves the energy barrier of the transition event, which is different for each event, the first event at the high temperature may not be the earliest event at the low temperature. TAD handles this by first generating a set of possible events from the current basin. After each event, the simulation is reflected backwards into the current basin. This is repeated until the stopping criterion is satisfied, at which point the event with the earliest low-temperature occurrence time is selected. The stopping criterion is that the confidence measure be greater than 1-*delta*. The confidence measure is the probability that no earlier low-temperature event will occur at some later time in the high-temperature simulation. hTST provides an lower bound for this probability, based on the user-specified minimum pre-exponential factor (reciprocal of *tmax*).

In order to estimate the energy barrier for each event, the TAD method invokes the *NEB* method. Each NEB replica runs on a partition of processors. The current NEB implementation in LAMMPS restricts you to having exactly one processor per replica. For more information, see the documentation for the *neb* command. In the current LAMMPS implementation of TAD, all the non-NEB TAD operations are performed on the first partition, while the other partitions remain idle. See the *Howto replica* doc page for further discussion of multi-replica simulations.

A TAD run has several stages, which are repeated each time an event is performed. The logic for a TAD run is as follows:

```
while (time remains):
  while (time < tstop):
```

(continues on next page)

(continued from previous page)

```
    until (event occurs):
      run dynamics for t_event steps
      quench
    run neb calculation using all replicas
    compute tlo from energy barrier
    update earliest event
    update tstop
    reflect back into current basin
  execute earliest event
```

Before this outer loop begins, the initial potential energy basin is identified by quenching (an energy minimization, see below) the initial state and storing the resulting coordinates for reference.

Inside the inner loop, dynamics is run continuously according to whatever integrator has been specified by the user, stopping every *t_event* steps to check if a transition event has occurred. This check is performed by quenching the system and comparing the resulting atom coordinates to the coordinates from the previous basin.

A quench is an energy minimization and is performed by whichever algorithm has been defined by the *min_style* command; its default is the CG minimizer. The tolerances and limits for each quench can be set by the *min* keyword. Note that typically, you do not need to perform a highly-converged minimization to detect a transition event.

The event check is performed by a compute with the specified *compute-ID*. Currently there is only one compute that works with the TAD command, which is the *compute event/displace* command. Other event-checking computes may be added. *Compute event/displace* checks whether any atom in the compute group has moved further than a specified threshold distance. If so, an "event" has occurred.

The NEB calculation is similar to that invoked by the *neb* command, except that the final state is generated internally, instead of being read in from a file. The style of minimization performed by NEB is determined by the *neb_style* keyword and must be a damped dynamics minimizer. The tolerances and limits for each NEB calculation can be set by the *neb* keyword. As discussed on the *neb*, it is often advantageous to use a larger timestep for NEB than for normal dynamics. Since the size of the timestep set by the *timestep* command is used by TAD for performing dynamics, there is a *neb_step* keyword which can be used to set a larger timestep for each NEB calculation if desired.

A key aspect of the TAD method is setting the stopping criterion appropriately. If this criterion is too conservative, then many events must be generated before one is finally executed. Conversely, if this criterion is too aggressive, high-entropy high-barrier events will be over-sampled, while low-entropy low-barrier events will be under-sampled. If the lowest pre-exponential factor is known fairly accurately, then it can be used to estimate *tmax*, and the value of *delta* can be set to the desired confidence level e.g. *delta* = 0.05 corresponds to 95% confidence. However, for systems where the dynamics are not well characterized (the most common case), it will be necessary to experiment with the values of *delta* and *tmax* to get a good trade-off between accuracy and performance.

A second key aspect is the choice of *t_hi*. A larger value greatly increases the rate at which new events are generated. However, too large a value introduces errors due to anharmonicity (not accounted for within hTST). Once again, for any given system, experimentation is necessary to determine the best value of *t_hi*.

Five kinds of output can be generated during a TAD run: event statistics, NEB statistics, thermodynamic output by each replica, dump files, and restart files.

Event statistics are printed to the screen and master log.lammps file each time an event is executed. The quantities are the timestep, CPU time, global event number *N*, local event number *M*, event status, energy barrier, time margin, *t_lo* and *delt_lo*. The timestep is the usual LAMMPS timestep, which corresponds to the high-temperature time at which the event was detected, in units of timestep. The CPU time is the total processor time since the start of the TAD run. The global event number *N* is a counter that increments with each executed event. The local event number *M* is a

counter that resets to zero upon entering each new basin. The event status is *E* when an event is executed, and is *D* for an event that is detected, while *DF* is for a detected event that is also the earliest (first) event at the low temperature.

The time margin is the ratio of the high temperature time in the current basin to the stopping time. This last number can be used to judge whether the stopping time is too short or too long (see above).

t_lo is the low-temperature event time when the current basin was entered, in units of timestep. del*t_lo* is the time of each detected event, measured relative to *t_lo*. *delt_lo* is equal to the high-temperature time since entering the current basin, scaled by an exponential factor that depends on the hi/lo temperature ratio and the energy barrier for that event.

On lines for executed events, with status *E*, the global event number is incremented by one, the local event number and time margin are reset to zero, while the global event number, energy barrier, and *delt_lo* match the last event with status *DF* in the immediately preceding block of detected events. The low-temperature event time *t_lo* is incremented by *delt_lo*.

NEB statistics are written to the file specified by the *neb_log* keyword. If the keyword value is "none", then no NEB statistics are printed out. The statistics are written every *Nevery* timesteps. See the *neb* command for a full description of the NEB statistics. When invoked from TAD, NEB statistics are never printed to the screen.

Because the NEB calculation must run on multiple partitions, LAMMPS produces additional screen and log files for each partition, e.g. log.lammps.0, log.lammps.1, etc. For the TAD command, these contain the thermodynamic output of each NEB replica. In addition, the log file for the first partition, log.lammps.0, will contain thermodynamic output from short runs and minimizations corresponding to the dynamics and quench operations, as well as a line for each new detected event, as described above.

After the TAD command completes, timing statistics for the TAD run are printed in each replica's log file, giving a breakdown of how much CPU time was spent in each stage (NEB, dynamics, quenching, etc).

Any *dump files* defined in the input script will be written to during a TAD run at timesteps when an event is executed. This means the requested dump frequency in the *dump* command is ignored. There will be one dump file (per dump command) created for all partitions. The atom coordinates of the dump snapshot are those of the minimum energy configuration resulting from quenching following the executed event. The timesteps written into the dump files correspond to the timestep at which the event occurred and NOT the clock. A dump snapshot corresponding to the initial minimum state used for event detection is written to the dump file at the beginning of each TAD run.

If the *restart* command is used, a single restart file for all the partitions is generated, which allows a TAD run to be continued by a new input script in the usual manner. The restart file is generated after an event is executed. The restart file contains a snapshot of the system in the new quenched state, including the event number and the low-temperature time. The restart frequency specified in the *restart* command is interpreted differently when performing a TAD run. It does not mean the timestep interval between restart files. Instead it means an event interval for executed events. Thus a frequency of 1 means write a restart file every time an event is executed. A frequency of 10 means write a restart file every 10th executed event. When an input script reads a restart file from a previous TAD run, the new script can be run on a different number of replicas or processors.

Note that within a single state, the dynamics will typically temporarily continue beyond the event that is ultimately chosen, until the stopping criterion is satisfied. When the event is eventually executed, the timestep counter is reset to the value when the event was detected. Similarly, after each quench and NEB minimization, the timestep counter is reset to the value at the start of the minimization. This means that the timesteps listed in the replica log files do not always increase monotonically. However, the timestep values printed to the master log file, dump files, and restart files are always monotonically increasing.

15.115.4 Restrictions

This command can only be used if LAMMPS was built with the REPLICA package. See the *Build package* doc page for more info.

N setting must be integer multiple of *t_event*.

Runs restarted from restart files written during a TAD run will only produce identical results if the user-specified integrator supports exact restarts. So *fix nvt* will produce an exact restart, but *fix langevin* will not.

This command cannot be used when any fixes are defined that keep track of elapsed time to perform time-dependent operations. Examples include the "ave" fixes such as *fix ave/chunk*. Also *fix dt/reset* and *fix deposit*.

15.115.5 Related commands

compute event/displace, *min_modify*, *min_style*, *run_style*, *minimize*, *temper*, *neb*, *prd*

15.115.6 Default

The option defaults are *min* = 0.1 0.1 40 50, *neb* = 0.01 100 100 10, *neb_style* = *quickmin*, *neb_step* = the same timestep set by the *timestep* command, and *neb_log* = "none".

(Voter2000) Sorensen and Voter, J Chem Phys, 112, 9599 (2000)

(Voter2002) Voter, Montalenti, Germann, Annual Review of Materials Research 32, 321 (2002).

15.116 temper command

15.116.1 Syntax

```
temper N M temp fix-ID seed1 seed2 index
```

- N = total # of timesteps to run
- M = attempt a tempering swap every this many steps
- temp = initial temperature for this ensemble
- fix-ID = ID of the fix that will control temperature during the run
- seed1 = random # seed used to decide on adjacent temperature to partner with
- seed2 = random # seed for Boltzmann factor in Metropolis swap
- index = which temperature (0 to N-1) I am simulating (optional)

15.116.2 Examples

```
temper 100000 100 $t tempfix 0 58728
temper 40000 100 $t tempfix 0 32285 $w
```

15.116.3 Description

Run a parallel tempering or replica exchange simulation using multiple replicas (ensembles) of a system. Two or more replicas must be used.

Each replica runs on a partition of one or more processors. Processor partitions are defined at run-time using the *-partition command-line switch*. Note that if you have MPI installed, you can run a multi-replica simulation with more replicas (partitions) than you have physical processors, e.g you can run a 10-replica simulation on one or two processors. You will simply not get the performance speed-up you would see with one or more physical processors per replica. See the *Howto replica* doc page for further discussion.

Each replica's temperature is controlled at a different value by a fix with *fix-ID* that controls temperature. Most thermostat fix styles (with and without included time integration) are supported. The command will print an error message and abort, if the chosen fix is unsupported. The desired temperature is specified by *temp*, which is typically a variable previously set in the input script, so that each partition is assigned a different temperature. See the *variable* command for more details. For example:

```
variable t world 300.0 310.0 320.0 330.0
fix myfix all nvt temp $t $t 100.0
temper 100000 100 $t myfix 3847 58382
```

would define 4 temperatures, and assign one of them to the thermostat used by each replica, and to the temper command.

As the tempering simulation runs for *N* timesteps, a temperature swap between adjacent ensembles will be attempted every *M* timesteps. If *seed1* is 0, then the swap attempts will alternate between odd and even pairings. If *seed1* is non-zero then it is used as a seed in a random number generator to randomly choose an odd or even pairing each time. Each attempted swap of temperatures is either accepted or rejected based on a Boltzmann-weighted Metropolis criterion which uses *seed2* in the random number generator.

As a tempering run proceeds, multiple log files and screen output files are created, one per replica. By default these files are named log.lammps.M and screen.M where M is the replica number from 0 to N-1, with N = # of replicas. See the *-log and -screen command-line swiches* for info on how to change these names.

The main screen and log file (log.lammps) will list information about which temperature is assigned to each replica at each thermodynamic output timestep. E.g. for a simulation with 16 replicas:

```
Running on 16 partitions of processors
Step T0 T1 T2 T3 T4 T5 T6 T7 T8 T9 T10 T11 T12 T13 T14 T15
0    0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
500  1 0 3 2 5 4 6 7 8 9 10 11 12 13 14 15
1000 2 0 4 1 5 3 6 7 8 9 10 11 12 14 13 15
1500 2 1 4 0 5 3 6 7 9 8 10 11 12 14 13 15
2000 2 1 3 0 6 4 5 7 10 8 9 11 12 14 13 15
2500 2 1 3 0 6 4 5 7 11 8 9 10 12 14 13 15
...
```

The column headings T0 to TN-1 mean which temperature is currently assigned to the replica 0 to N-1. Thus the columns represent replicas and the value in each column is its temperature (also numbered 0 to N-1). For example, a 0 in the 4th column (column T3, step 2500) means that the 4th replica is assigned temperature 0, i.e. the lowest temperature. You can verify this time sequence of temperature assignments for the Nth replica by comparing the

Nth column of screen output to the thermodynamic data in the corresponding log.lammps.N or screen.N files as time proceeds.

You can have each replica create its own dump file in the following manner:

```
variable rep world 0 1 2 3 4 5 6 7
dump 1 all atom 1000 dump.temper.$rep
```

Note: Each replica's dump file will contain a continuous trajectory for its atoms where the temperature varies over time as swaps take place involving that replica. If you want a series of dump files, each with snapshots (from all replicas) that are all at a single temperature, then you will need to post-process the dump files using the information from the log.lammps file. E.g. you could produce one dump file with snapshots at 300K (from all replicas), another with snapshots at 310K, etc. Note that these new dump files will not contain "continuous trajectories" for individual atoms, because two successive snapshots (in time) may be from different replicas. The reorder_remd_traj python script can do the reordering for you (and additionally also calculated configurational log-weights of trajectory snapshots in the canonical ensemble). The script can be found in the tools/replica directory while instructions on how to use it is available in doc/Tools (in brief) and as a README file in tools/replica (in detail).

The last argument *index* in the temper command is optional and is used when restarting a tempering run from a set of restart files (one for each replica) which had previously swapped to new temperatures. The *index* value (from 0 to N-1, where N is the # of replicas) identifies which temperature the replica was simulating on the timestep the restart files were written. Obviously, this argument must be a variable so that each partition has the correct value. Set the variable to the *N* values listed in the log file for the previous run for the replica temperatures at that timestep. For example if the log file listed the following for a simulation with 5 replicas:

```
500000 2 4 0 1 3
```

then a setting of

```
variable w world 2 4 0 1 3
```

would be used to restart the run with a tempering command like the example above with $w as the last argument.

15.116.4 Restrictions

This command can only be used if LAMMPS was built with the REPLICA package. See the *Build package* doc page for more info.

15.116.5 Related commands

variable, *prd*, *neb*

Default: none

15.117 temper/grem command

15.117.1 Syntax

```
temper/grem N M lambda fix-ID thermostat-ID seed1 seed2 index
```

- N = total # of timesteps to run
- M = attempt a tempering swap every this many steps
- lambda = initial lambda for this ensemble
- fix-ID = ID of *fix grem*
- thermostat-ID = ID of the thermostat that controls kinetic temperature
- seed1 = random # seed used to decide on adjacent temperature to partner with
- seed2 = random # seed for Boltzmann factor in Metropolis swap
- index = which temperature (0 to N-1) I am simulating (optional)

15.117.2 Examples

```
temper/grem 100000 1000 $lambda fxgREM fxnvt 0 58728
temper/grem 40000 100 $lambda fxgREM fxnpt 0 32285 $walkers
```

15.117.3 Description

Run a parallel tempering or replica exchange simulation in LAMMPS partition mode using multiple generalized replicas (ensembles) of a system defined by *fix grem*, which stands for the generalized replica exchange method (gREM) originally developed by *(Kim)*. It uses non-Boltzmann ensembles to sample over first order phase transitions. The is done by defining replicas with an enthalpy dependent effective temperature

Two or more replicas must be used. See the *temper* command for an explanation of how to run replicas on multiple partitions of one or more processors.

This command is a modification of the *temper* command and has the same dependencies, restraints, and input variables which are discussed there in greater detail.

Instead of temperature, this command performs replica exchanges in lambda as per the generalized ensemble enforced by *fix grem*. The desired lambda is specified by *lambda*, which is typically a variable previously set in the input script, so that each partition is assigned a different temperature. See the *variable* command for more details. For example:

```
variable lambda world 400 420 440 460
fix fxnvt all nvt temp 300.0 300.0 100.0
fix fxgREM all grem $lambda -0.05 -50000 fxnvt
temper 100000 100 $lambda fxgREM fxnvt 3847 58382
```

would define 4 lambdas with constant kinetic temperature but unique generalized temperature, and assign one of them to *fix grem* used by each replica, and to the grem command.

As the gREM simulation runs for *N* timesteps, a swap between adjacent ensembles will be attempted every *M* timesteps. If *seed1* is 0, then the swap attempts will alternate between odd and even pairings. If *seed1* is non-zero then it is used as a seed in a random number generator to randomly choose an odd or even pairing each time. Each attempted swap of temperatures is either accepted or rejected based on a Metropolis criterion, derived for gREM by *(Kim)*, which uses *seed2* in the random number generator.

File management works identical to the *temper* command. Dump files created by this fix contain continuous trajectories and require post-processing to obtain per-replica information.

The last argument *index* in the grem command is optional and is used when restarting a run from a set of restart files (one for each replica) which had previously swapped to new lambda. This is done using a variable. For example if the log file listed the following for a simulation with 5 replicas:

```
500000 2 4 0 1 3
```

then a setting of

```
variable walkers world 2 4 0 1 3
```

would be used to restart the run with a grem command like the example above with $*walkers* as the last argument. This functionality is identical to *temper*.

15.117.4 Restrictions

This command can only be used if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

This command must be used with *fix grem*.

15.117.5 Related commands

fix grem, *temper*, *variable*

Default: none

(Kim) Kim, Keyes, Straub, J Chem Phys, 132, 224107 (2010).

15.118 temper/npt command

15.118.1 Syntax

```
temper/npt  N M temp fix-ID seed1 seed2 pressure index
```

- N = total # of timesteps to run
- M = attempt a tempering swap every this many steps
- temp = initial temperature for this ensemble
- fix-ID = ID of the fix that will control temperature and pressure during the run
- seed1 = random # seed used to decide on adjacent temperature to partner with
- seed2 = random # seed for Boltzmann factor in Metropolis swap
- pressure = setpoint pressure for the ensemble
- index = which temperature (0 to N-1) I am simulating (optional)

15.118.2 Examples

```
temper/npt 100000 100 $t nptfix 0 58728 1
temper/npt 2500000 1000 300 nptfix  0 32285 $p
temper/npt 5000000 2000 $t nptfix 0 12523 1 $w
```

15.118.3 Description

Run a parallel tempering or replica exchange simulation using multiple replicas (ensembles) of a system in the isothermal-isobaric (NPT) ensemble. The command temper/npt works like *temper* but requires running replicas in the NPT ensemble instead of the canonical (NVT) ensemble and allows for pressure to be set in the ensembles. These multiple ensembles can run in parallel at different temperatures or different pressures. The acceptance criteria for temper/npt is specific to the NPT ensemble and can be found in references *(Okabe)* and *(Mori)*.

Apart from the difference in acceptance criteria and the specification of pressure, this command works much like the *temper* command. See the documentation on *temper* for information on how the parallel tempering is handled in general.

15.118.4 Restrictions

This command can only be used if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

This command should be used with a fix that maintains the isothermal-isobaric (NPT) ensemble.

15.118.5 Related commands

temper, *variable*, *fix_npt*

Default: none

(Okabe) T. Okabe, M. Kawata, Y. Okamoto, M. Masuhiro, Chem. Phys. Lett., 335, 435-439 (2001).

(Mori) Y. Mori, Y. Okamoto, J. Phys. Soc. Jpn., 7, 074003 (2010).

15.119 thermo command

15.119.1 Syntax

```
thermo N
```

- N = output thermodynamics every N timesteps
- N can be a variable (see below)

15.119.2 Examples

```
thermo 100
```

15.119.3 Description

Compute and print thermodynamic info (e.g. temperature, energy, pressure) on timesteps that are a multiple of N and at the beginning and end of a simulation. A value of 0 will only print thermodynamics at the beginning and end.

The content and format of what is printed is controlled by the *thermo_style* and *thermo_modify* commands.

Instead of a numeric value, N can be specified as an *equal-style variable*, which should be specified as v_name, where name is the variable name. In this case, the variable is evaluated at the beginning of a run to determine the next timestep at which thermodynamic info will be written out. On that timestep, the variable will be evaluated again to determine the next timestep, etc. Thus the variable should return timestep values. See the stagger() and logfreq() and stride() math functions for *equal-style variables*, as examples of useful functions to use in this context. Other similar math functions could easily be added as options for *equal-style variables*.

For example, the following commands will output thermodynamic info at timesteps 0,10,20,30,100,200,300,1000,2000,etc:

```
variable        s equal logfreq(10,3,10)
thermo          v_s
```

15.119.4 Restrictions

none

15.119.5 Related commands

thermo_style, *thermo_modify*

15.119.6 Default

```
thermo 0
```

15.120 thermo_modify command

15.120.1 Syntax

```
thermo_modify keyword value ...
```

- one or more keyword/value pairs may be listed

```
keyword = lost or lost/bond or norm or flush or line or format or temp or␣
↪press:l
  lost value = error or warn or ignore
  lost/bond value = error or warn or ignore
  norm value = yes or no
```

```
flush value = yes or no
line value = one or multi
format values = line string, int string, float string, M string, or none
  string = C-style format string
  M = integer from 1 to N, where N = # of quantities being output
temp value = compute ID that calculates a temperature
press value = compute ID that calculates a pressure
```

15.120.2 Examples

```
thermo_modify lost ignore flush yes
thermo_modify temp myTemp format 3 %15.8g
thermo_modify temp myTemp format line "%ld %g %g %15.8g"
thermo_modify line multi format float %g
```

15.120.3 Description

Set options for how thermodynamic information is computed and printed by LAMMPS.

Note: These options apply to the currently defined thermo style. When you specify a *thermo_style* command, all thermodynamic settings are restored to their default values, including those previously reset by a thermo_modify command. Thus if your input script specifies a thermo_style command, you should use the thermo_modify command after it.

The *lost* keyword determines whether LAMMPS checks for lost atoms each time it computes thermodynamics and what it does if atoms are lost. An atom can be "lost" if it moves across a non-periodic simulation box *boundary* or if it moves more than a box length outside the simulation domain (or more than a processor sub-domain length) before reneighboring occurs. The latter case is typically due to bad dynamics, e.g. too large a timestep or huge forces and velocities. If the value is *ignore*, LAMMPS does not check for lost atoms. If the value is *error* or *warn*, LAMMPS checks and either issues an error or warning. The code will exit with an error and continue with a warning. A warning will only be issued once, the first time an atom is lost. This can be a useful debugging option.

The *lost/bond* keyword determines whether LAMMPS throws an error or not if an atom in a bonded interaction (bond, angle, etc) cannot be found when it creates bonded neighbor lists. By default this is a fatal error. However in some scenarios it may be desirable to only issue a warning or ignore it and skip the computation of the missing bond, angle, etc. An example would be when gas molecules in a vapor are drifting out of the box through a fixed boundary condition (see the *boundary* command). In this case one atom may be deleted before the rest of the molecule is, on a later timestep.

The *norm* keyword determines whether various thermodynamic output values are normalized by the number of atoms or not, depending on whether it is set to *yes* or *no*. Different unit styles have different defaults for this setting (see below). Even if *norm* is set to *yes*, a value is only normalized if it is an "extensive" quantity, meaning that it scales with the number of atoms in the system. For the thermo keywords described by the doc page for the *thermo_style* command, all energy-related keywords are extensive, such as *pe* or *ebond* or *enthalpy*. Other keywords such as *temp* or *press* are "intensive" meaning their value is independent (in a statistical sense) of the number of atoms in the system and thus are never normalized. For thermodynamic output values extracted from fixes and computes in a *thermo_style custom* command, the doc page for the individual *fix* or *compute* lists whether the value is "extensive" or "intensive" and thus whether it is normalized. Thermodynamic output values calculated by a variable formula are assumed to be "intensive" and thus are never normalized. You can always include a divide by the number of atoms in the variable formula if this is not the case.

The *flush* keyword invokes a flush operation after thermodynamic info is written to the log file. This insures the output in that file is current (no buffering by the OS), even if LAMMPS halts before the simulation completes.

The *line* keyword determines whether thermodynamics will be output as a series of numeric values on one line or in a multi-line format with 3 quantities with text strings per line and a dashed-line header containing the timestep and CPU time. This modify option overrides the *one* and *multi* thermo_style settings.

The *format* keyword can be used to change the default numeric format of any of quantities the *thermo_style* command outputs. All the specified format strings are C-style formats, e.g. as used by the C/C++ printf() command. The *line* keyword takes a single argument which is the format string for the entire line of thermo output, with N fields, which you must enclose in quotes if it is more than one field. The *int* and *float* keywords take a single format argument and are applied to all integer or floating-point quantities output. The setting for *M string* also takes a single format argument which is used for the Mth value output in each line, e.g. the 5th column is output in high precision for "format 5 %20.15g".

The *format* keyword can be used multiple times. The precedence is that for each value in a line of output, the *M* format (if specified) is used, else the *int* or *float* setting (if specified) is used, else the *line* setting (if specified) for that value is used, else the default setting is used. A setting of *none* clears all previous settings, reverting all values to their default format.

Note: The thermo output values *step* and *atoms* are stored internally as 8-byte signed integers, rather than the usual 4-byte signed integers. When specifying the *format int* option you can use a "%d"-style format identifier in the format string and LAMMPS will convert this to the corresponding 8-byte form when it is applied to those keywords. However, when specifying the *line* option or *format M string* option for *step* and *natoms*, you should specify a format string appropriate for an 8-byte signed integer, e.g. one with "%ld".

The *temp* keyword is used to determine how thermodynamic temperature is calculated, which is used by all thermo quantities that require a temperature ("temp", "press", "ke", "etotal", "enthalpy", "pxx", etc). The specified compute ID must have been previously defined by the user via the *compute* command and it must be a style of compute that calculates a temperature. As described in the *thermo_style* command, thermo output uses a default compute for temperature with ID = *thermo_temp*. This option allows the user to override the default.

The *press* keyword is used to determine how thermodynamic pressure is calculated, which is used by all thermo quantities that require a pressure ("press", "enthalpy", "pxx", etc). The specified compute ID must have been previously defined by the user via the *compute* command and it must be a style of compute that calculates a pressure. As described in the *thermo_style* command, thermo output uses a default compute for pressure with ID = *thermo_press*. This option allows the user to override the default.

Note: If both the *temp* and *press* keywords are used in a single thermo_modify command (or in two separate commands), then the order in which the keywords are specified is important. Note that a *pressure compute* defines its own temperature compute as an argument when it is specified. The *temp* keyword will override this (for the pressure compute being used by thermodynamics), but only if the *temp* keyword comes after the *press* keyword. If the *temp* keyword comes before the *press* keyword, then the new pressure compute specified by the *press* keyword will be unaffected by the *temp* setting.

15.120.4 Restrictions

none

15.120.5 Related commands

thermo, *thermo_style*

15.120.6 Default

The option defaults are lost = error, norm = yes for unit style of *lj*, norm = no for unit style of *real* and *metal*, flush = no, and temp/press = compute IDs defined by thermo_style.

The defaults for the line and format options depend on the thermo style. For styles "one" and "custom", the line and format defaults are "one", "%8d", and "%12.8g". For style "multi", the line and format defaults are "multi", "%8d", and "%14.4f".

15.121 thermo_style command

15.121.1 Syntax

```
thermo_style style args
```

- style = *one* or *multi* or *custom*
- args = list of arguments for a particular style

```
one args = none
multi args = none
custom args = list of keywords
  possible keywords = step, elapsed, elaplong, dt, time,
                      cpu, tpcpu, spcpu, cpuremain, part, timeremain,
                      atoms, temp, press, pe, ke, etotal, enthalpy,
                      evdwl, ecoul, epair, ebond, eangle, edihed, eimp,
                      emol, elong, etail,
                      vol, density, lx, ly, lz, xlo, xhi, ylo, yhi, zlo,␣
 ↪zhi,
                      xy, xz, yz, xlat, ylat, zlat,
                      bonds, angles, dihedrals, impropers,
                      pxx, pyy, pzz, pxy, pxz, pyz,
                      fmax, fnorm, nbuild, ndanger,
                      cella, cellb, cellc, cellalpha, cellbeta, cellgamma,
                      c_ID, c_ID[I], c_ID[I][J],
                      f_ID, f_ID[I], f_ID[I][J],
                      v_name, v_name[I]
    step = timestep
    elapsed = timesteps since start of this run
    elaplong = timesteps since start of initial run in a series of runs
    dt = timestep size
    time = simulation time
    cpu = elapsed CPU time in seconds since start of this run
```

```
   tpcpu = time per CPU second
   spcpu = timesteps per CPU second
   cpuremain = estimated CPU time remaining in run
   part = which partition (0 to Npartition-1) this is
   timeremain = remaining time in seconds on timer timeout.
   atoms = # of atoms
   temp = temperature
   press = pressure
   pe = total potential energy
   ke = kinetic energy
   etotal = total energy (pe + ke)
   enthalpy = enthalpy (etotal + press*vol)
   evdwl = van der Waals pairwise energy (includes etail)
   ecoul = Coulombic pairwise energy
   epair = pairwise energy (evdwl + ecoul + elong)
   ebond = bond energy
   eangle = angle energy
   edihed = dihedral energy
   eimp = improper energy
   emol = molecular energy (ebond + eangle + edihed + eimp)
   elong = long-range kspace energy
   etail = van der Waals energy long-range tail correction
   vol = volume
   density = mass density of system
   lx,ly,lz = box lengths in x,y,z
   xlo,xhi,ylo,yhi,zlo,zhi = box boundaries
   xy,xz,yz = box tilt for triclinic (non-orthogonal) simulation boxes
   xlat,ylat,zlat = lattice spacings as calculated by lattice command
   bonds,angles,dihedrals,impropers = # of these interactions defined
   pxx,pyy,pzz,pxy,pxz,pyz = 6 components of pressure tensor
   fmax = max component of force on any atom in any dimension
   fnorm = length of force vector for all atoms
   nbuild = # of neighbor list builds
   ndanger = # of dangerous neighbor list builds
   cella,cellb,cellc = periodic cell lattice constants a,b,c
   cellalpha, cellbeta, cellgamma = periodic cell angles alpha,beta,gamma
   c_ID = global scalar value calculated by a compute with ID
   c_ID[I] = Ith component of global vector calculated by a compute with␣
↪ID, I can include wildcard (see below)
   c_ID[I][J] = I,J component of global array calculated by a compute␣
↪with ID
   f_ID = global scalar value calculated by a fix with ID
   f_ID[I] = Ith component of global vector calculated by a fix with ID,␣
↪I can include wildcard (see below)
   f_ID[I][J] = I,J component of global array calculated by a fix with ID
   v_name = value calculated by an equal-style variable with name
   v_name[I] = value calculated by a vector-style variable with name
```

15.121.2 Examples

```
thermo_style multi
thermo_style custom step temp pe etotal press vol
thermo_style custom step temp etotal c_myTemp v_abc
thermo_style custom step temp etotal c_myTemp[*] v_abc
```

15.121.3 Description

Set the style and content for printing thermodynamic data to the screen and log file.

Style *one* prints a one-line summary of thermodynamic info that is the equivalent of "thermo_style custom step temp epair emol etotal press". The line contains only numeric values.

Style *multi* prints a multiple-line listing of thermodynamic info that is the equivalent of "thermo_style custom etotal ke temp pe ebond eangle edihed eimp evdwl ecoul elong press". The listing contains numeric values and a string ID for each quantity.

Style *custom* is the most general setting and allows you to specify which of the keywords listed above you want printed on each thermodynamic timestep. Note that the keywords c_ID, f_ID, v_name are references to *computes*, *fixes*, and equal-style *variables* that have been defined elsewhere in the input script or can even be new styles which users have added to LAMMPS. See the *Modify* doc page for details on the latter. Thus the *custom* style provides a flexible means of outputting essentially any desired quantity as a simulation proceeds.

All styles except *custom* have *vol* appended to their list of outputs if the simulation box volume changes during the simulation.

The values printed by the various keywords are instantaneous values, calculated on the current timestep. Time-averaged quantities, which include values from previous timesteps, can be output by using the f_ID keyword and accessing a fix that does time-averaging such as the *fix ave/time* command.

Options invoked by the *thermo_modify* command can be used to set the one- or multi-line format of the print-out, the normalization of thermodynamic output (total values versus per-atom values for extensive quantities (ones which scale with the number of atoms in the system), and the numeric precision of each printed value.

Note: When you use a "thermo_style" command, all thermodynamic settings are restored to their default values, including those previously set by a *thermo_modify* command. Thus if your input script specifies a thermo_style command, you should use the thermo_modify command after it.

Several of the thermodynamic quantities require a temperature to be computed: "temp", "press", "ke", "etotal", "enthalpy", "pxx", etc. By default this is done by using a *temperature* compute which is created when LAMMPS starts up, as if this command had been issued:

```
compute thermo_temp all temp
```

See the *compute temp* command for details. Note that the ID of this compute is *thermo_temp* and the group is *all*. You can change the attributes of this temperature (e.g. its degrees-of-freedom) via the *compute_modify* command. Alternatively, you can directly assign a new compute (that calculates temperature) which you have defined, to be used for calculating any thermodynamic quantity that requires a temperature. This is done via the *thermo_modify* command.

Several of the thermodynamic quantities require a pressure to be computed: "press", "enthalpy", "pxx", etc. By default this is done by using a *pressure* compute which is created when LAMMPS starts up, as if this command had been issued:

```
compute thermo_press all pressure thermo_temp
```

See the *compute pressure* command for details. Note that the ID of this compute is *thermo_press* and the group is *all*. You can change the attributes of this pressure via the *compute_modify* command. Alternatively, you can directly assign a new compute (that calculates pressure) which you have defined, to be used for calculating any thermodynamic quantity that requires a pressure. This is done via the *thermo_modify* command.

Several of the thermodynamic quantities require a potential energy to be computed: "pe", "etotal", "ebond", etc. This is done by using a *pe* compute which is created when LAMMPS starts up, as if this command had been issued:

```
compute thermo_pe all pe
```

See the *compute pe* command for details. Note that the ID of this compute is *thermo_pe* and the group is *all*. You can change the attributes of this potential energy via the *compute_modify* command.

The kinetic energy of the system *ke* is inferred from the temperature of the system with $\frac{1}{2}k_BT$ of energy for each degree of freedom. Thus, using different *compute commands* for calculating temperature, via the *thermo_modify temp* command, may yield different kinetic energies, since different computes that calculate temperature can subtract out different non-thermal components of velocity and/or include different degrees of freedom (translational, rotational, etc).

The potential energy of the system *pe* will include contributions from fixes if the *fix_modify thermo* option is set for a fix that calculates such a contribution. For example, the *fix wall/lj93* fix calculates the energy of atoms interacting with the wall. See the doc pages for "individual fixes" to see which ones contribute.

A long-range tail correction *etail* for the van der Waals pairwise energy will be non-zero only if the *pair_modify tail* option is turned on. The *etail* contribution is included in *evdwl*, *epair*, *pe*, and *etotal*, and the corresponding tail correction to the pressure is included in *press* and *pxx*, *pyy*, etc.

The *step*, *elapsed*, and *elaplong* keywords refer to timestep count. *Step* is the current timestep, or iteration count when a *minimization* is being performed. *Elapsed* is the number of timesteps elapsed since the beginning of this run. *Elaplong* is the number of timesteps elapsed since the beginning of an initial run in a series of runs. See the *start* and *stop* keywords for the *run* for info on how to invoke a series of runs that keep track of an initial starting time. If these keywords are not used, then *elapsed* and *elaplong* are the same value.

The *dt* keyword is the current timestep size in time *units*. The *time* keyword is the current elapsed simulation time, also in time *units*, which is simply (step*dt) if the timestep size has not changed and the timestep has not been reset. If the timestep has changed (e.g. via *fix dt/reset*) or the timestep has been reset (e.g. via the "reset_timestep" command), then the simulation time is effectively a cumulative value up to the current point.

The *cpu* keyword is elapsed CPU seconds since the beginning of this run. The *tpcpu* and *spcpu* keywords are measures of how fast your simulation is currently running. The *tpcpu* keyword is simulation time per CPU second, where simulation time is in time *units*. E.g. for metal units, the *tpcpu* value would be picoseconds per CPU second. The *spcpu* keyword is the number of timesteps per CPU second. Both quantities are on-the-fly metrics, measured relative to the last time they were invoked. Thus if you are printing out thermodynamic output every 100 timesteps, the two keywords will continually output the time and timestep rate for the last 100 steps. The *tpcpu* keyword does not attempt to track any changes in timestep size, e.g. due to using the *fix dt/reset* command.

The *cpuremain* keyword estimates the CPU time remaining in the current run, based on the time elapsed thus far. It will only be a good estimate if the CPU time/timestep for the rest of the run is similar to the preceding timesteps. On the initial timestep the value will be 0.0 since there is no history to estimate from. For a minimization run performed by the "minimize" command, the estimate is based on the *maxiter* parameter, assuming the minimization will proceed for the maximum number of allowed iterations.

The *part* keyword is useful for multi-replica or multi-partition simulations to indicate which partition this output and this file corresponds to, or for use in a *variable* to append to a filename for output specific to this partition. See discussion of the *-partition command-line switch* for details on running in multi-partition mode.

The *timeremain* keyword returns the remaining seconds when a timeout has been configured via the *timer timeout* command. If the timeout timer is inactive, the value of this keyword is 0.0 and if the timer is expired, it is negative. This allows for example to exit loops cleanly, if the timeout is expired with:

```
if "$(timeremain) < 0.0" then "quit 0"
```

The *fmax* and *fnorm* keywords are useful for monitoring the progress of an *energy minimization*. The *fmax* keyword calculates the maximum force in any dimension on any atom in the system, or the infinity-norm of the force vector for the system. The *fnorm* keyword calculates the 2-norm or length of the force vector.

The *nbuild* and *ndanger* keywords are useful for monitoring neighbor list builds during a run. Note that both these values are also printed with the end-of-run statistics. The *nbuild* keyword is the number of re-builds during the current run. The *ndanger* keyword is the number of re-builds that LAMMPS considered potentially "dangerous". If atom movement triggered neighbor list rebuilding (see the *neigh_modify* command), then dangerous reneighborings are those that were triggered on the first timestep atom movement was checked for. If this count is non-zero you may wish to reduce the delay factor to insure no force interactions are missed by atoms moving beyond the neighbor skin distance before a rebuild takes place.

The keywords *cella*, *cellb*, *cellc*, *cellalpha*, *cellbeta*, *cellgamma*, correspond to the usual crystallographic quantities that define the periodic unit cell of a crystal. See the *Howto triclinic* doc page for a geometric description of triclinic periodic cells, including a precise definition of these quantities in terms of the internal LAMMPS cell dimensions *lx*, *ly*, *lz*, *yz*, *xz*, *xy*.

For output values from a compute or fix, the bracketed index I used to index a vector, as in *c_ID[I]* or *f_ID[I]*, can be specified using a wildcard asterisk with the index to effectively specify multiple values. This takes the form "*" or "*n" or "n*" or "m*n". If N = the size of the vector (for *mode* = scalar) or the number of columns in the array (for *mode* = vector), then an asterisk with no numeric values means all indices from 1 to N. A leading asterisk means all indices from 1 to n (inclusive). A trailing asterisk means all indices from n to N (inclusive). A middle asterisk means all indices from m to n (inclusive).

Using a wildcard is the same as if the individual elements of the vector had been listed one by one. E.g. these 2 thermo_style commands are equivalent, since the *compute temp* command creates a global vector with 6 values.

```
compute myTemp all temp
thermo_style custom step temp etotal c_myTemp[*]
thermo_style custom step temp etotal &
             c_myTemp[1] c_myTemp[2] c_myTemp[3] &
             c_myTemp[4] c_myTemp[5] c_myTemp[6]
```

The *c_ID* and *c_ID[I]* and *c_ID[I][J]* keywords allow global values calculated by a compute to be output. As discussed on the *compute* doc page, computes can calculate global, per-atom, or local values. Only global values can be referenced by this command. However, per-atom compute values for an individual atom can be referenced in a *variable* and the variable referenced by thermo_style custom, as discussed below. See the discussion above for how the I in *c_ID[I]* can be specified with a wildcard asterisk to effectively specify multiple values from a global compute vector.

The ID in the keyword should be replaced by the actual ID of a compute that has been defined elsewhere in the input script. See the *compute* command for details. If the compute calculates a global scalar, vector, or array, then the keyword formats with 0, 1, or 2 brackets will reference a scalar value from the compute.

Note that some computes calculate "intensive" global quantities like temperature; others calculate "extensive" global quantities like kinetic energy that are summed over all atoms in the compute group. Intensive quantities are printed

directly without normalization by thermo_style custom. Extensive quantities may be normalized by the total number of atoms in the simulation (NOT the number of atoms in the compute group) when output, depending on the *thermo_modify norm* option being used.

The *f_ID* and *f_ID[I]* and *f_ID[I][J]* keywords allow global values calculated by a fix to be output. As discussed on the *fix* doc page, fixes can calculate global, per-atom, or local values. Only global values can be referenced by this command. However, per-atom fix values can be referenced for an individual atom in a *variable* and the variable referenced by thermo_style custom, as discussed below. See the discussion above for how the I in *f_ID[I]* can be specified with a wildcard asterisk to effectively specify multiple values from a global fix vector.

The ID in the keyword should be replaced by the actual ID of a fix that has been defined elsewhere in the input script. See the *fix* command for details. If the fix calculates a global scalar, vector, or array, then the keyword formats with 0, 1, or 2 brackets will reference a scalar value from the fix.

Note that some fixes calculate "intensive" global quantities like timestep size; others calculate "extensive" global quantities like energy that are summed over all atoms in the fix group. Intensive quantities are printed directly without normalization by thermo_style custom. Extensive quantities may be normalized by the total number of atoms in the simulation (NOT the number of atoms in the fix group) when output, depending on the *thermo_modify norm* option being used.

The *v_name* keyword allow the current value of a variable to be output. The name in the keyword should be replaced by the variable name that has been defined elsewhere in the input script. Only equal-style and vector-style variables can be referenced; the latter requires a bracketed term to specify the Ith element of the vector calculated by the variable. However, an atom-style variable can be referenced for an individual atom by an equal-style variable and that variable referenced. See the *variable* command for details. Variables of style *equal* and *vector* and *atom* define a formula which can reference per-atom properties or thermodynamic keywords, or they can invoke other computes, fixes, or variables when evaluated, so this is a very general means of creating thermodynamic output.

Note that equal-style and vector-style variables are assumed to produce "intensive" global quantities, which are thus printed as-is, without normalization by thermo_style custom. You can include a division by "natoms" in the variable formula if this is not the case.

15.121.4 Restrictions

This command must come after the simulation box is defined by a *read_data*, *read_restart*, or *create_box* command.

15.121.5 Related commands

thermo, *thermo_modify*, *fix_modify*, *compute temp*, *compute pressure*

15.121.6 Default

```
thermo_style one
```

15.122 third_order command

15.122.1 Syntax

```
third_order group-ID style delta args keyword value ...
```

- group-ID = ID of group of atoms to displace
- style = *regular* or *eskm*
- delta = finite different displacement length (distance units)
- one or more keyword/arg pairs may be appended

```
keyword = file or binary
  file name = name of output file for the third order tensor
  binary arg = yes or no or gzip
```

15.122.2 Examples

```
third_order 1 regular 0.000001
third_order 1 eskm 0.000001
third_order 3 regular 0.00004 file third_order.dat
third_order 5 eskm 0.00000001 file third_order.dat binary yes
```

15.122.3 Description

Calculate the third order force constant tensor by finite difference of the selected group,

$$\Phi_{ijk}^{\alpha\beta\gamma} = \frac{\partial^3 U}{\partial x_{i,\alpha} \partial x_{j,\beta} \partial x_{k,\gamma}}$$

where Phi is the third order force constant tensor.

The output of the command is the tensor, three elements at a time. The three elements correspond to the three gamma elements for a specific i/alpha/j/beta/k. The initial five numbers are i, alpha, j, beta, and k respectively.

If the style eskm is selected, the tensor will be using energy units of 10 J/mol. These units conform to eskm style from the dynamical_matrix command, which will simplify operations using dynamical matrices with third order tensors.

15.122.4 Restrictions

The command collects a 9 times the number of atoms in the group on every single MPI rank, so the memory requirements can be very significant for large systems.

This command is part of the USER-PHONON package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

15.122.5 Related commands

fix phonon dynamical_matrix

15.122.6 Default

The default settings are file = "third_order.dat", binary = no

15.123 timer command

15.123.1 Syntax

```
timer args
```

- *args* = one or more of *off* or *loop* or *normal* or *full* or *sync* or *nosync* or *timeout* or *every*

```
off = do not collect or print any timing information
loop = collect only the total time for the simulation loop
normal = collect timer information broken down by sections (default)
full = like normal but also include CPU and thread utilization
sync = explicitly synchronize MPI tasks between sections
nosync = do not synchronize MPI tasks between sections (default)
timeout elapse = set wall time limit to elapse
every Ncheck = perform timeout check every Ncheck steps
```

15.123.2 Examples

```
timer full sync
timer timeout 2:00:00 every 100
timer loop
```

15.123.3 Description

Select the level of detail at which LAMMPS performs its CPU timings. Multiple keywords can be specified with the *timer* command. For keywords that are mutually exclusive, the last one specified takes precedence.

During a simulation run LAMMPS collects information about how much time is spent in different sections of the code and thus can provide information for determining performance and load imbalance problems. This can be done at different levels of detail and accuracy. For more information about the timing output, see the *Run output* doc page.

The *off* setting will turn all time measurements off. The *loop* setting will only measure the total time for a run and not collect any detailed per section information. With the *normal* setting, timing information for portions of the

timestep (pairwise calculations, neighbor list construction, output, etc) are collected as well as information about load imbalances for those sections across processors. The *full* setting adds information about CPU utilization and thread utilization, when multi-threading is enabled.

With the *sync* setting, all MPI tasks are synchronized at each timer call which measures load imbalance for each section more accurately, though it can also slow down the simulation by prohibiting overlapping independent computations on different MPI ranks Using the *nosync* setting (which is the default) turns this synchronization off.

With the *timeout* keyword a wall time limit can be imposed, that affects the *run* and *minimize* commands. This can be convenient when calculations have to comply with execution time limits, e.g. when running under a batch system when you want to maximize the utilization of the batch time slot, especially for runs where the time per timestep varies much and thus it becomes difficult to predict how many steps a simulation can perform for a given wall time limit. This also applies for difficult to converge minimizations. The timeout *elapse* value should be somewhat smaller than the maximum wall time requested from the batch system, as there is usually some overhead to launch jobs, and it is advisable to write out a restart after terminating a run due to a timeout.

The timeout timer starts when the command is issued. When the time limit is reached, the run or energy minimization will exit on the next step or iteration that is a multiple of the *Ncheck* value which can be set with the *every* keyword. Default is checking every 10 steps. After the timer timeout has expired all subsequent run or minimize commands in the input script will be skipped. The remaining time or timer status can be accessed with the *thermo* variable *timeremain*, which will be zero, if the timeout is inactive (default setting), it will be negative, if the timeout time is expired and positive if there is time remaining and in this case the value of the variable are the number of seconds remaining.

When the *timeout* key word is used a second time, the timer is restarted with a new time limit. The timeout *elapse* value can be specified as *off* or *unlimited* to impose a no timeout condition (which is the default). The *elapse* setting can be specified as a single number for seconds, two numbers separated by a colon (MM:SS) for minutes and seconds, or as three numbers separated by colons for hours, minutes, and seconds (H:MM:SS).

The *every* keyword sets how frequently during a run or energy minimization the wall clock will be checked. This check count applies to the outer iterations or time steps during minimizations or *r-RESPA runs*, respectively. Checking for timeout too often, can slow a calculation down. Checking too infrequently can make the timeout measurement less accurate, with the run being stopped later than desired.

Note: Using the *full* and *sync* options provides the most detailed and accurate timing information, but can also have a negative performance impact due to the overhead of the many required system calls. It is thus recommended to use these settings only when testing tests to identify performance bottlenecks. For calculations with few atoms or a very large number of processors, even the *normal* setting can have a measurable negative performance impact. In those cases you can just use the *loop* or *off* setting.

15.123.4 Restrictions

none

15.123.5 Related commands

run post no, *kspace_modify fftbench*

15.123.6 Default

```
timer normal nosync
timer timeout off
timer every 10
```

15.124 timestep command

15.124.1 Syntax

```
timestep dt
```

- dt = timestep size (time units)

15.124.2 Examples

```
timestep 2.0
timestep 0.003
```

15.124.3 Description

Set the timestep size for subsequent molecular dynamics simulations. See the *units* command for the time units associated with each choice of units that LAMMPS supports.

The default value for the timestep size also depends on the choice of units for the simulation; see the default values below.

When the *run style* is *respa*, dt is the timestep for the outer loop (largest) timestep.

15.124.4 Restrictions

none

15.124.5 Related commands

fix dt/reset, *run*, *run_style* respa, *units*

15.124.6 Default

choice of *units*	time units	default timestep size
lj	tau	0.005 tau
real	fmsec	1.0 fmsec
metal	psec	0.001 psec
si	sec	1.0e-8 sec (10 nsec)
cgs	sec	1.0e-8 sec (10 nsec)
electron	fmsec	0.001 fmsec
micro	usec	2.0 usec
nano	nsec	0.00045 nsec

15.125 uncompute command

15.125.1 Syntax

```
uncompute compute-ID
```

- compute-ID = ID of a previously defined compute

15.125.2 Examples

```
uncompute 2
uncompute lower-boundary
```

15.125.3 Description

Delete a compute that was previously defined with a *compute* command. This also wipes out any additional changes made to the compute via the *compute_modify* command.

15.125.4 Restrictions

none

15.125.5 Related commands

compute

Default: none

15.126 undump command

15.126.1 Syntax

```
undump dump-ID
```

- dump-ID = ID of previously defined dump

15.126.2 Examples

```
undump mine
undump 2
```

15.126.3 Description

Turn off a previously defined dump so that it is no longer active. This closes the file associated with the dump.

15.126.4 Restrictions

none

15.126.5 Related commands

dump

Default: none

15.127 unfix command

15.127.1 Syntax

```
unfix fix-ID
```

- fix-ID = ID of a previously defined fix

15.127.2 Examples

```
unfix 2
unfix lower-boundary
```

15.127.3 Description

Delete a fix that was previously defined with a *fix* command. This also wipes out any additional changes made to the fix via the *fix_modify* command.

15.127.4 Restrictions

none

15.127.5 Related commands

fix

Default: none

15.128 units command

15.128.1 Syntax

```
units style
```

- style = *lj* or *real* or *metal* or *si* or *cgs* or *electron* or *micro* or *nano*

15.128.2 Examples

```
units metal
units lj
```

15.128.3 Description

This command sets the style of units used for a simulation. It determines the units of all quantities specified in the input script and data file, as well as quantities output to the screen, log file, and dump files. Typically, this command is used at the very beginning of an input script.

For all units except *lj*, LAMMPS uses physical constants from www.physics.nist.gov. For the definition of Kcal in real units, LAMMPS uses the thermochemical calorie = 4.184 J.

The choice you make for units simply sets some internal conversion factors within LAMMPS. This means that any simulation you perform for one choice of units can be duplicated with any other unit setting LAMMPS supports. In this context "duplicate" means the particles will have identical trajectories and all output generated by the simulation will be identical. This will be the case for some number of timesteps until round-off effects accumulate, since the conversion factors for two different unit systems are not identical to infinite precision.

To perform the same simulation in a different set of units you must change all the unit-based input parameters in your input script and other input files (data file, potential files, etc) correctly to the new units. And you must correctly convert all output from the new units to the old units when comparing to the original results. That is often not simple to do.

For style *lj*, all quantities are unitless. Without loss of generality, LAMMPS sets the fundamental quantities mass, σ, ϵ, and the Boltzmann constant $k_B = 1$. The masses, distances, energies you specify are multiples of these fundamental values. The formulas relating the reduced or unitless quantity (with an asterisk) to the same quantity with units is also given. Thus you can use the mass & σ & ϵ values for a specific material and convert the results from a unitless LJ simulation into physical quantities.

- mass = mass or *m*
- distance = σ, where $x^* = \frac{x}{\sigma}$
- time = τ, where $\tau^* = \tau\sqrt{\frac{\epsilon}{m\sigma^2}}$
- energy = ϵ, where $E^* = \frac{E}{\epsilon}$
- velocity = $\frac{\sigma}{\tau}$, where $v^* = v\frac{\tau}{\sigma}$
- force = $\frac{\epsilon}{\sigma}$, where $f^* = f\frac{\sigma}{\epsilon}$
- torque = ϵ, where $t^* = \frac{t}{\epsilon}$
- temperature = reduced LJ temperature, where $T^* = \frac{Tk_B}{\epsilon}$
- pressure = reduced LJ pressure, where $p^* = p\frac{\sigma^3}{\epsilon}$
- dynamic viscosity = reduced LJ viscosity, where $\eta^* = \eta\frac{\sigma^3}{\epsilon\tau}$
- charge = reduced LJ charge, where $q^* = q\frac{1}{\sqrt{4\pi\varepsilon_0\sigma\epsilon}}$
- dipole = reduced LJ dipole, moment where $\mu^* = \mu\frac{1}{\sqrt{4\pi\varepsilon_0\sigma^3\epsilon}}$
- electric field = force/charge, where $E^* = E\frac{\sqrt{4\pi\varepsilon_0\sigma\epsilon}\sigma}{\epsilon}$
- density = mass/volume, where $\rho^* = \rho\sigma^{dim}$

Note that for LJ units, the default mode of thermodynamic output via the *thermo_style* command is to normalize all extensive quantities by the number of atoms. E.g. potential energy is extensive because it is summed over atoms, so it is output as energy/atom. Temperature is intensive since it is already normalized by the number of atoms, so it is output as-is. This behavior can be changed via the *thermo_modify norm* command.

For style *real*, these are the units:

- mass = grams/mole
- distance = Angstroms
- time = femtoseconds
- energy = Kcal/mole
- velocity = Angstroms/femtosecond
- force = Kcal/mole-Angstrom
- torque = Kcal/mole
- temperature = Kelvin
- pressure = atmospheres
- dynamic viscosity = Poise

- charge = multiple of electron charge (1.0 is a proton)
- dipole = charge*Angstroms
- electric field = volts/Angstrom
- density = gram/cm^dim

For style *metal*, these are the units:

- mass = grams/mole
- distance = Angstroms
- time = picoseconds
- energy = eV
- velocity = Angstroms/picosecond
- force = eV/Angstrom
- torque = eV
- temperature = Kelvin
- pressure = bars
- dynamic viscosity = Poise
- charge = multiple of electron charge (1.0 is a proton)
- dipole = charge*Angstroms
- electric field = volts/Angstrom
- density = gram/cm^dim

For style *si*, these are the units:

- mass = kilograms
- distance = meters
- time = seconds
- energy = Joules
- velocity = meters/second
- force = Newtons
- torque = Newton-meters
- temperature = Kelvin
- pressure = Pascals
- dynamic viscosity = Pascal*second
- charge = Coulombs (1.6021765e-19 is a proton)
- dipole = Coulombs*meters
- electric field = volts/meter
- density = kilograms/meter^dim

For style *cgs*, these are the units:

- mass = grams

- distance = centimeters
- time = seconds
- energy = ergs
- velocity = centimeters/second
- force = dynes
- torque = dyne-centimeters
- temperature = Kelvin
- pressure = dyne/cm^2 or barye = 1.0e-6 bars
- dynamic viscosity = Poise
- charge = statcoulombs or esu (4.8032044e-10 is a proton)
- dipole = statcoul-cm = 10^18 debye
- electric field = statvolt/cm or dyne/esu
- density = grams/cm^dim

For style *electron*, these are the units:

- mass = atomic mass units
- distance = Bohr
- time = femtoseconds
- energy = Hartrees
- velocity = Bohr/atomic time units [1.03275e-15 seconds]
- force = Hartrees/Bohr
- temperature = Kelvin
- pressure = Pascals
- charge = multiple of electron charge (1.0 is a proton)
- dipole moment = Debye
- electric field = volts/cm

For style *micro*, these are the units:

- mass = picograms
- distance = micrometers
- time = microseconds
- energy = picogram-micrometer^2/microsecond^2
- velocity = micrometers/microsecond
- force = picogram-micrometer/microsecond^2
- torque = picogram-micrometer^2/microsecond^2
- temperature = Kelvin
- pressure = picogram/(micrometer-microsecond^2)
- dynamic viscosity = picogram/(micrometer-microsecond)

- charge = picocoulombs (1.6021765e-7 is a proton)
- dipole = picocoulomb-micrometer
- electric field = volt/micrometer
- density = picograms/micrometer^dim

For style *nano*, these are the units:

- mass = attograms
- distance = nanometers
- time = nanoseconds
- energy = attogram-nanometer^2/nanosecond^2
- velocity = nanometers/nanosecond
- force = attogram-nanometer/nanosecond^2
- torque = attogram-nanometer^2/nanosecond^2
- temperature = Kelvin
- pressure = attogram/(nanometer-nanosecond^2)
- dynamic viscosity = attogram/(nanometer-nanosecond)
- charge = multiple of electron charge (1.0 is a proton)
- dipole = charge-nanometer
- electric field = volt/nanometer
- density = attograms/nanometer^dim

The units command also sets the timestep size and neighbor skin distance to default values for each style:

- For style *lj* these are dt = 0.005 tau and skin = 0.3 sigma.
- For style *real* these are dt = 1.0 femtoseconds and skin = 2.0 Angstroms.
- For style *metal* these are dt = 0.001 picoseconds and skin = 2.0 Angstroms.
- For style *si* these are dt = 1.0e-8 seconds and skin = 0.001 meters.
- For style *cgs* these are dt = 1.0e-8 seconds and skin = 0.1 centimeters.
- For style *electron* these are dt = 0.001 femtoseconds and skin = 2.0 Bohr.
- For style *micro* these are dt = 2.0 microseconds and skin = 0.1 micrometers.
- For style *nano* these are dt = 0.00045 nanoseconds and skin = 0.1 nanometers.

15.128.4 Restrictions

This command cannot be used after the simulation box is defined by a *read_data* or *create_box* command.

Related commands: none

15.128.5 Default

```
units lj
```

15.129 variable command

15.129.1 Syntax

```
variable name style args ...
```

- name = name of variable to define
- style = *delete* or *index* or *loop* or *world* or *universe* or *uloop* or *string* or *format* or *getenv* or *file* or *atomfile* or *python* or *internal* or *equal* or *vector* or *atom*

```
delete = no args
index args = one or more strings
loop args = N
  N = integer size of loop, loop from 1 to N inclusive
loop args = N pad
  N = integer size of loop, loop from 1 to N inclusive
  pad = all values will be same length, e.g. 001, 002, ..., 100
loop args = N1 N2
  N1,N2 = loop from N1 to N2 inclusive
loop args = N1 N2 pad
  N1,N2 = loop from N1 to N2 inclusive
  pad = all values will be same length, e.g. 050, 051, ..., 100
world args = one string for each partition of processors
universe args = one or more strings
uloop args = N
  N = integer size of loop
uloop args = N pad
  N = integer size of loop
  pad = all values will be same length, e.g. 001, 002, ..., 100
string arg = one string
format args = vname fstr
  vname = name of equal-style variable to evaluate
  fstr = C-style format string
getenv arg = one string
file arg = filename
atomfile arg = filename
python arg = function
internal arg = numeric value
equal or vector or atom args = one formula containing numbers, thermo␣
↪keywords, math operations, group functions, atom values and vectors,␣
↪compute/fix/variable references
  numbers = 0.0, 100, -5.4, 2.8e-4, etc
  constants = PI, version, on, off, true, false, yes, no
  thermo keywords = vol, ke, press, etc from thermo_style
  math operators = (), -x, x+y, x-y, x*y, x/y, x^y, x%y,
                   x == y, x != y, x < y, x <= y, x > y, x >= y, x && y,␣
↪x || y, x |^ y, !x
```

```
 math functions = sqrt(x), exp(x), ln(x), log(x), abs(x),
                  sin(x), cos(x), tan(x), asin(x), acos(x), atan(x),␣
↪atan2(y,x),
                  random(x,y,z), normal(x,y,z), ceil(x), floor(x),␣
↪round(x)
                  ramp(x,y), stagger(x,y), logfreq(x,y,z), logfreq2(x,y,
↪z),
                  logfreq3(x,y,z), stride(x,y,z), stride2(x,y,z,a,b,c),
                  vdisplace(x,y), swiggle(x,y,z), cwiggle(x,y,z)
 group functions = count(group), mass(group), charge(group),
                   xcm(group,dim), vcm(group,dim), fcm(group,dim),
                   bound(group,dir), gyration(group), ke(group),
                   angmom(group,dim), torque(group,dim),
                   inertia(group,dimdim), omega(group,dim)
 region functions = count(group,region), mass(group,region),␣
↪charge(group,region),
                   xcm(group,dim,region), vcm(group,dim,region),␣
↪fcm(group,dim,region),
                   bound(group,dir,region), gyration(group,region),␣
↪ke(group,reigon),
                   angmom(group,dim,region), torque(group,dim,region),
                   inertia(group,dimdim,region), omega(group,dim,region)
 special functions = sum(x), min(x), max(x), ave(x), trap(x), slope(x),␣
↪gmask(x), rmask(x), grmask(x,y), next(x)
 feature functions = is_active(category,feature,exact), is_
↪defined(category,id,exact)
 atom value = id[i], mass[i], type[i], mol[i], x[i], y[i], z[i], vx[i],␣
↪vy[i], vz[i], fx[i], fy[i], fz[i], q[i]
 atom vector = id, mass, type, mol, x, y, z, vx, vy, vz, fx, fy, fz, q
 compute references = c_ID, c_ID[i], c_ID[i][j], C_ID, C_ID[i]
 fix references = f_ID, f_ID[i], f_ID[i][j], F_ID, F_ID[i]
 variable references = v_name, v_name[i]
```

15.129.2 Examples

```
variable x index run1 run2 run3 run4 run5 run6 run7 run8
variable LoopVar loop $n
variable beta equal temp/3.0
variable b1 equal x[234]+0.5*vol
variable b1 equal "x[234] + 0.5*vol"
variable b equal xcm(mol1,x)/2.0
variable b equal c_myTemp
variable b atom x*y/vol
variable foo string myfile
variable foo internal 3.5
variable myPy python increase
variable f file values.txt
variable temp world 300.0 310.0 320.0 ${Tfinal}
variable x universe 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
variable x uloop 15 pad
variable str format x %.6g
variable x delete
```

15.129.3 Description

This command assigns one or more strings to a variable name for evaluation later in the input script or during a simulation.

Variables can thus be useful in several contexts. A variable can be defined and then referenced elsewhere in an input script to become part of a new input command. For variable styles that store multiple strings, the *next* command can be used to increment which string is assigned to the variable. Variables of style *equal* store a formula which when evaluated produces a single numeric value which can be output either directly (see the *print*, *fix print*, and *run every* commands) or as part of thermodynamic output (see the *thermo_style* command), or used as input to an averaging fix (see the *fix ave/time* command). Variables of style *vector* store a formula which produces a vector of such values which can be used as input to various averaging fixes, or elements of which can be part of thermodynamic output. Variables of style *atom* store a formula which when evaluated produces one numeric value per atom which can be output to a dump file (see the *dump custom* command) or used as input to an averaging fix (see the *fix ave/chunk* and *fix ave/atom* commands). Variables of style *atomfile* can be used anywhere in an input script that atom-style variables are used; they get their per-atom values from a file rather than from a formula. Variables of style *python* can be hooked to Python functions using code you provide, so that the variable gets its value from the evaluation of the Python code. Variables of style *internal* are used by a few commands which set their value directly.

Note: As discussed on the *Commands parse* doc page, an input script can use "immediate" variables, specified as $(formula) with parenthesis, where the formula has the same syntax as equal-style variables described on this page. This is a convenient way to evaluate a formula immediately without using the variable command to define a named variable and then evaluate that variable. See below for a more detailed discussion of this feature.

In the discussion that follows, the "name" of the variable is the arbitrary string that is the 1st argument in the variable command. This name can only contain alphanumeric characters and underscores. The "string" is one or more of the subsequent arguments. The "string" can be simple text as in the 1st example above, it can contain other variables as in the 2nd example, or it can be a formula as in the 3rd example. The "value" is the numeric quantity resulting from evaluation of the string. Note that the same string can generate different values when it is evaluated at different times during a simulation.

Note: When an input script line is encountered that defines a variable of style *equal* or *vector* or *atom* or *python* that contains a formula or Python code, the formula is NOT immediately evaluated. It will be evaluated every time when the variable is **used** instead. If you simply want to evaluate a formula in place you can use as so-called. See the section below about "Immediate Evaluation of Variables" for more details on the topic. This is also true of a *format* style variable since it evaluates another variable when it is invoked.

Variables of style *equal* and *vector* and *atom* can be used as inputs to various other commands which evaluate their formulas as needed, e.g. at different timesteps during a *run*.

Variables of style *internal* can be used in place of an equal-style variable, except by commands that set the value stored by the internal-style variable. Thus any command that states it can use an equal-style variable as an argument, can also use an internal-style variable. This means that when the command evaluates the variable, it will use the value set (internally) by another command.

Variables of style *python* can be used in place of an equal-style variable so long as the associated Python function, as defined by the *python* command, returns a numeric value. Thus any command that states it can use an equal-style variable as an argument, can also use such a python-style variable. This means that when the LAMMPS command evaluates the variable, the Python function will be executed.

Note: When a variable command is encountered in the input script and the variable name has already been specified, the command is ignored. This means variables can NOT be re-defined in an input script (with two exceptions, read further). This is to allow an input script to be processed multiple times without resetting the variables; see the *jump* or

include commands. It also means that using the *command-line switch* -var will override a corresponding index variable setting in the input script.

There are two exceptions to this rule. First, variables of style *string*, *getenv*, *internal*, *equal*, *vector*, *atom*, and *python* ARE redefined each time the command is encountered. This allows these style of variables to be redefined multiple times in an input script. In a loop, this means the formula associated with an *equal* or *atom* style variable can change if it contains a substitution for another variable, e.g. $x or v_x.

Second, as described below, if a variable is iterated on to the end of its list of strings via the *next* command, it is removed from the list of active variables, and is thus available to be re-defined in a subsequent variable command. The *delete* style does the same thing.

The *Commands parse* doc page explains how occurrences of a variable name in an input script line are replaced by the variable's string. The variable name can be referenced as $x if the name "x" is a single character, or as ${LoopVar} if the name "LoopVar" is one or more characters.

As described below, for variable styles *index*, *loop*, *file*, *universe*, and *uloop*, which string is assigned to a variable can be incremented via the *next* command. When there are no more strings to assign, the variable is exhausted and a flag is set that causes the next *jump* command encountered in the input script to be skipped. This enables the construction of simple loops in the input script that are iterated over and then exited from.

As explained above, an exhausted variable can be re-used in an input script. The *delete* style also removes the variable, the same as if it were exhausted, allowing it to be redefined later in the input script or when the input script is looped over. This can be useful when breaking out of a loop via the *if* and *jump* commands before the variable would become exhausted. For example,

```
label       loop
variable    a loop 5
print       "A = $a"
if          "$a > 2" then "jump in.script break"
next        a
jump        in.script loop
label       break
variable    a delete
```

This section describes how all the various variable styles are defined and what they store. Except for the *equal* and *vector* and *atom* styles, which are explained in the next section.

Many of the styles store one or more strings. Note that a single string can contain spaces (multiple words), if it is enclosed in quotes in the variable command. When the variable is substituted for in another input script command, its returned string will then be interpreted as multiple arguments in the expanded command.

For the *index* style, one or more strings are specified. Initially, the 1st string is assigned to the variable. Each time a *next* command is used with the variable name, the next string is assigned. All processors assign the same string to the variable.

Index style variables with a single string value can also be set by using the *command-line switch -var*.

The *loop* style is identical to the *index* style except that the strings are the integers from 1 to N inclusive, if only one argument N is specified. This allows generation of a long list of runs (e.g. 1000) without having to list N strings in the input script. Initially, the string "1" is assigned to the variable. Each time a *next* command is used with the variable name, the next string ("2", "3", etc) is assigned. All processors assign the same string to the variable. The *loop* style can also be specified with two arguments N1 and N2. In this case the loop runs from N1 to N2 inclusive, and the string N1 is initially assigned to the variable. N1 <= N2 and N2 >= 0 is required.

For the *world* style, one or more strings are specified. There must be one string for each processor partition or "world". LAMMPS can be run with multiple partitions via the *-partition command-line switch*. This variable command assigns one string to each world. All processors in the world are assigned the same string. The next command cannot be used with *equal* style variables, since there is only one value per world. This style of variable is useful when you wish to run different simulations on different partitions, or when performing a parallel tempering simulation (see the *temper* command), to assign different temperatures to different partitions.

For the *universe* style, one or more strings are specified. There must be at least as many strings as there are processor partitions or "worlds". LAMMPS can be run with multiple partitions via the *-partition command-line switch*. This variable command initially assigns one string to each world. When a *next* command is encountered using this variable, the first processor partition to encounter it, is assigned the next available string. This continues until all the variable strings are consumed. Thus, this command can be used to run 50 simulations on 8 processor partitions. The simulations will be run one after the other on whatever partition becomes available, until they are all finished. *Universe* style variables are incremented using the files "tmp.lammps.variable" and "tmp.lammps.variable.lock" which you will see in your directory during such a LAMMPS run.

The *uloop* style is identical to the *universe* style except that the strings are the integers from 1 to N. This allows generation of long list of runs (e.g. 1000) without having to list N strings in the input script.

For the *string* style, a single string is assigned to the variable. Two differences between this style and using the *index* style exist: a variable with *string* style can be redefined, e.g. by another command later in the input script, or if the script is read again in a loop. The other difference is that *string* performs variable substitution even if the string parameter is quoted.

For the *format* style, an equal-style variable is specified along with a C-style format string, e.g. "%f" or "%.10g", which must be appropriate for formatting a double-precision floating-point value. The default format is "%.15g". This variable style allows an equal-style variable to be formatted precisely when it is evaluated.

If you simply wish to print a variable value with desired precision to the screen or logfile via the *print* or *fix print* commands, you can also do this by specifying an "immediate" variable with a trailing colon and format string, as part of the string argument of those commands. This is explained on the *Commands parse* doc page.

For the *getenv* style, a single string is assigned to the variable which should be the name of an environment variable. When the variable is evaluated, it returns the value of the environment variable, or an empty string if it not defined. This style of variable can be used to adapt the behavior of LAMMPS input scripts via environment variable settings, or to retrieve information that has been previously stored with the *shell putenv* command. Note that because environment variable settings are stored by the operating systems, they persist beyond a *clear* command.

For the *file* style, a filename is provided which contains a list of strings to assign to the variable, one per line. The strings can be numeric values if desired. See the discussion of the next() function below for equal-style variables, which will convert the string of a file-style variable into a numeric value in a formula.

When a file-style variable is defined, the file is opened and the string on the first line is read and stored with the variable. This means the variable can then be evaluated as many times as desired and will return that string. There are two ways to cause the next string from the file to be read: use the *next* command or the next() function in an equal- or atom-style variable, as discussed below.

The rules for formatting the file are as follows. A comment character "#" can be used anywhere on a line; text starting with the comment character is stripped. Blank lines are skipped. The first "word" of a non-blank line, delimited by white-space, is the "string" assigned to the variable.

For the *atomfile* style, a filename is provided which contains one or more sets of values, to assign on a per-atom basis to the variable. The format of the file is described below.

When an atomfile-style variable is defined, the file is opened and the first set of per-atom values are read and stored with the variable. This means the variable can then be evaluated as many times as desired and will return those values. There are two ways to cause the next set of per-atom values from the file to be read: use the *next* command or the next() function in an atom-style variable, as discussed below.

The rules for formatting the file are as follows. Each time a set of per-atom values is read, a non-blank line is searched for in the file. A comment character "#" can be used anywhere on a line; text starting with the comment character is stripped. Blank lines are skipped. The first "word" of a non-blank line, delimited by white-space, is read as the count N of per-atom lines to immediately follow. N can be the total number of atoms in the system, or only a subset. The next N lines have the following format

```
ID value
```

where ID is an atom ID and value is the per-atom numeric value that will be assigned to that atom. IDs can be listed in any order.

Note: Every time a set of per-atom lines is read, the value for all atoms is first set to 0.0. Thus values for atoms whose ID does not appear in the set, will remain 0.0.

For the *python* style a Python function name is provided. This needs to match a function name specified in a *python* command which returns a value to this variable as defined by its *return* keyword. For example these two commands would be self-consistent:

```
variable foo python myMultiply
python myMultiply return v_foo format f file funcs.py
```

The two commands can appear in either order so long as both are specified before the Python function is invoked for the first time.

Each time the variable is evaluated, the associated Python function is invoked, and the value it returns is also returned by the variable. Since the Python function can use other LAMMPS variables as input, or query interal LAMMPS quantities to perform its computation, this means the variable can return a different value each time it is evaluated.

The type of value stored in the variable is determined by the *format* keyword of the *python* command. It can be an integer (i), floating point (f), or string (s) value. As mentioned above, if it is a numeric value (integer or floating point), then the python-style variable can be used in place of an equal-style variable anywhere in an input script, e.g. as an argument to another command that allows for equal-style variables.

For the *internal* style a numeric value is provided. This value will be assigned to the variable until a LAMMPS command sets it to a new value. There are currently only two LAMMPS commands that require *internal* variables as inputs, because they reset them: *create_atoms* and *fix controller*. As mentioned above, an internal-style variable can be used in place of an equal-style variable anywhere else in an input script, e.g. as an argument to another command that allows for equal-style variables.

For the *equal* and *vector* and *atom* styles, a single string is specified which represents a formula that will be evaluated afresh each time the variable is used. If you want spaces in the string, enclose it in double quotes so the parser will treat it as a single argument. For *equal*-style variables the formula computes a scalar quantity, which becomes the value of the variable whenever it is evaluated. For *vector*-style variables the formula must compute a vector of quantities, which becomes the value of the variable whenever it is evaluated. The calculated vector can be on length one, but it cannot be a simple scalar value like that produced by an equal-style compute. I.e. the formula for a vector-style variable must have at least one quantity in it that refers to a global vector produced by a compute, fix, or other vector-style variable. For *atom*-style variables the formula computes one quantity for each atom whenever it is evaluated.

Note that *equal*, *vector*, and *atom* variables can produce different values at different stages of the input script or at different times during a run. For example, if an *equal* variable is used in a *fix print* command, different values could be printed each timestep it was invoked. If you want a variable to be evaluated immediately, so that the result is stored by the variable instead of the string, see the section below on "Immediate Evaluation of Variables".

The next command cannot be used with *equal* or *vector* or *atom* style variables, since there is only one string.

The formula for an *equal*, *vector*, or *atom* variable can contain a variety of quantities. The syntax for each kind of quantity is simple, but multiple quantities can be nested and combined in various ways to build up formulas of arbitrary complexity. For example, this is a valid (though strange) variable formula:

```
variable x equal "pe + c_MyTemp / vol^(1/3)"
```

Specifically, a formula can contain numbers, constants, thermo keywords, math operators, math functions, group functions, region functions, atom values, atom vectors, compute references, fix references, and references to other variables.

Number	0.2, 100, 1.0e20, -15.4, etc
Constant	PI, version, on, off, true, false, yes, no
Thermo keywords	vol, pe, ebond, etc
Math operators	(), -x, x+y, x-y, x*y, x/y, x^y, x%y, x == y, x != y, x < y, x <= y, x > y, x >= y, x && y, x || y, x |^ y, !x
Math functions	sqrt(x), exp(x), ln(x), log(x), abs(x), sin(x), cos(x), tan(x), asin(x), acos(x), atan(x), atan2(y,x), random(x,y,z), normal(x,y,z), ceil(x), floor(x), round(x), ramp(x,y), stagger(x,y), logfreq(x,y,z), logfreq2(x,y,z), logfreq3(x,y,z), stride(x,y,z), stride2(x,y,z,a,b,c), vdisplace(x,y), swiggle(x,y,z), cwiggle(x,y,z)
Group functions	count(ID), mass(ID), charge(ID), xcm(ID,dim), vcm(ID,dim), fcm(ID,dim), bound(ID,dir), gyration(ID), ke(ID), angmom(ID,dim), torque(ID,dim), inertia(ID,dimdim), omega(ID,dim)
Region functions	count(ID,IDR), mass(ID,IDR), charge(ID,IDR), xcm(ID,dim,IDR), vcm(ID,dim,IDR), fcm(ID,dim,IDR), bound(ID,dir,IDR), gyration(ID,IDR), ke(ID,IDR), angmom(ID,dim,IDR), torque(ID,dim,IDR), inertia(ID,dimdim,IDR), omega(ID,dim,IDR)
Special functions	sum(x), min(x), max(x), ave(x), trap(x), slope(x), gmask(x), rmask(x), grmask(x,y), next(x)
Atom values	id[i], mass[i], type[i], mol[i], x[i], y[i], z[i], vx[i], vy[i], vz[i], fx[i], fy[i], fz[i], q[i]
Atom vectors	id, mass, type, mol, x, y, z, vx, vy, vz, fx, fy, fz, q
Compute references	c_ID, c_ID[i], c_ID[i][j], C_ID, C_ID[i]
Fix references	f_ID, f_ID[i], f_ID[i][j], F_ID, F_ID[i]
Other variables	v_name, v_name[i]

Most of the formula elements produce a scalar value. Some produce a global or per-atom vector of values. Global vectors can be produced by computes or fixes or by other vector-style variables. Per-atom vectors are produced by atom vectors, compute references that represent a per-atom vector, fix references that represent a per-atom vector,

and variables that are atom-style variables. Math functions that operate on scalar values produce a scalar value; math function that operate on global or per-atom vectors do so element-by-element and produce a global or per-atom vector.

A formula for equal-style variables cannot use any formula element that produces a global or per-atom vector. A formula for a vector-style variable can use formula elements that produce either a scalar value or a global vector value, but cannot use a formula element that produces a per-atom vector. A formula for an atom-style variable can use formula elements that produce either a scalar value or a per-atom vector, but not one that produces a global vector. Atom-style variables are evaluated by other commands that define a *group* on which they operate, e.g. a *dump* or *compute* or *fix* command. When they invoke the atom-style variable, only atoms in the group are included in the formula evaluation. The variable evaluates to 0.0 for atoms not in the group.

Numbers, constants, and thermo keywords

Numbers can contain digits, scientific notation (3.0e20,3.0e-20,3.0E20,3.0E-20), and leading minus signs.

Constants are set at compile time and cannot be changed. *PI* will return the number 3.14159265358979323846; *on*, *true* or *yes* will return 1.0; *off*, *false* or *no* will return 0.0; *version* will return a numeric version code of the current LAMMPS version (e.g. version 2 Sep 2015 will return the number 20150902). The corresponding value for newer versions of LAMMPS will be larger, for older versions of LAMMPS will be smaller. This can be used to have input scripts adapt automatically to LAMMPS versions, when non-backwards compatible syntax changes are introduced. Here is an illustrative example (which will not work, since the *version* has been introduced more recently):

```
if $(version<20140513) then "communicate vel yes" else "comm_modify vel yes"
```

The thermo keywords allowed in a formula are those defined by the *thermo_style custom* command. Thermo keywords that require a *compute* to calculate their values such as "temp" or "press", use computes stored and invoked by the *thermo_style* command. This means that you can only use those keywords in a variable if the style you are using with the thermo_style command (and the thermo keywords associated with that style) also define and use the needed compute. Note that some thermo keywords use a compute indirectly to calculate their value (e.g. the enthalpy keyword uses temp, pe, and pressure). If a variable is evaluated directly in an input script (not during a run), then the values accessed by the thermo keyword must be current. See the discussion below about "Variable Accuracy".

Math Operators

Math operators are written in the usual way, where the "x" and "y" in the examples can themselves be arbitrarily complex formulas, as in the examples above. In this syntax, "x" and "y" can be scalar values or per-atom vectors. For example, "ke/natoms" is the division of two scalars, where "vy+vz" is the element-by-element sum of two per-atom vectors of y and z velocities.

Operators are evaluated left to right and have the usual C-style precedence: unary minus and unary logical NOT operator "!" have the highest precedence, exponentiation "^" is next; multiplication and division and the modulo operator "%" are next; addition and subtraction are next; the 4 relational operators "<", "<=", ">", and ">=" are next; the two remaining relational operators "==" and "!=" are next; then the logical AND operator "&&"; and finally the logical OR operator "||" and logical XOR (exclusive or) operator "|^" have the lowest precedence. Parenthesis can be used to group one or more portions of a formula and/or enforce a different order of evaluation than what would occur with the default precedence.

Note: Because a unary minus is higher precedence than exponentiation, the formula "-2^2" will evaluate to 4, not -4. This convention is compatible with some programming languages, but not others. As mentioned, this behavior can be easily overridden with parenthesis; the formula "-(2^2)" will evaluate to -4.

The 6 relational operators return either a 1.0 or 0.0 depending on whether the relationship between x and y is TRUE or FALSE. For example the expression x<10.0 in an atom-style variable formula will return 1.0 for all atoms whose x-coordinate is less than 10.0, and 0.0 for the others. The logical AND operator will return 1.0 if both its arguments are non-zero, else it returns 0.0. The logical OR operator will return 1.0 if either of its arguments is non-zero, else it returns 0.0. The logical XOR operator will return 1.0 if one of its arguments is zero and the other non-zero, else it returns 0.0. The logical NOT operator returns 1.0 if its argument is 0.0, else it returns 0.0.

These relational and logical operators can be used as a masking or selection operation in a formula. For example, the number of atoms whose properties satisfy one or more criteria could be calculated by taking the returned per-atom vector of ones and zeroes and passing it to the *compute reduce* command.

Math Functions

Math functions are specified as keywords followed by one or more parenthesized arguments "x", "y", "z", each of which can themselves be arbitrarily complex formulas. In this syntax, the arguments can represent scalar values or global vectors or per-atom vectors. In the latter case, the math operation is performed on each element of the vector. For example, "sqrt(natoms)" is the sqrt() of a scalar, where "sqrt(y*z)" yields a per-atom vector with each element being the sqrt() of the product of one atom's y and z coordinates.

Most of the math functions perform obvious operations. The ln() is the natural log; log() is the base 10 log.

The random(x,y,z) function takes 3 arguments: x = lo, y = hi, and z = seed. It generates a uniform random number between lo and hi. The normal(x,y,z) function also takes 3 arguments: x = mu, y = sigma, and z = seed. It generates a Gaussian variate centered on mu with variance sigma^2. In both cases the seed is used the first time the internal random number generator is invoked, to initialize it. For equal-style and vector-style variables, every processor uses the same seed so that they each generate the same sequence of random numbers. For atom-style variables, a unique seed is created for each processor, based on the specified seed. This effectively generates a different random number for each atom being looped over in the atom-style variable.

Note: Internally, there is just one random number generator for all equal-style and vector-style variables and another one for all atom-style variables. If you define multiple variables (of each style) which use the random() or normal() math functions, then the internal random number generators will only be initialized once, which means only one of the specified seeds will determine the sequence of generated random numbers.

The ceil(), floor(), and round() functions are those in the C math library. Ceil() is the smallest integer not less than its argument. Floor() if the largest integer not greater than its argument. Round() is the nearest integer to its argument.

The ramp(x,y) function uses the current timestep to generate a value linearly interpolated between the specified x,y values over the course of a run, according to this formula:

```
value = x + (y-x) * (timestep-startstep) / (stopstep-startstep)
```

The run begins on startstep and ends on stopstep. Startstep and stopstep can span multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

The stagger(x,y) function uses the current timestep to generate a new timestep. X,y > 0 and x > y are required. The generated timesteps increase in a staggered fashion, as the sequence x,x+y,2x,2x+y,3x,3x+y,etc. For any current timestep, the next timestep in the sequence is returned. Thus if stagger(1000,100) is used in a variable by the *dump_modify every* command, it will generate the sequence of output timesteps:

```
100,1000,1100,2000,2100,3000,etc
```

The logfreq(x,y,z) function uses the current timestep to generate a new timestep. X,y,z > 0 and y < z are required. The generated timesteps are on a base-z logarithmic scale, starting with x, and the y value is how many

of the z-1 possible timesteps within one logarithmic interval are generated. I.e. the timesteps follow the sequence x,2x,3x,...y*x,x*z,2x*z,3x*z,...y*x*z,x*z^2,2x*z^2,etc. For any current timestep, the next timestep in the sequence is returned. Thus if logfreq(100,4,10) is used in a variable by the *dump_modify every* command, it will generate this sequence of output timesteps:

```
100,200,300,400,1000,2000,3000,4000,10000,20000,etc
```

The logfreq2(x,y,z) function is similar to logfreq, except a single logarithmic interval is divided into y equally-spaced timesteps and all of them are output. Y < z is not required. Thus, if logfreq2(100,18,10) is used in a variable by the *dump_modify every* command, then the interval between 100 and 1000 is divided as 900/18 = 50 steps, and it will generate the sequence of output timesteps:

```
100,150,200,...950,1000,1500,2000,...9500,10000,15000,etc
```

The logfreq3(x,y,z) function generates y points between x and z (inclusive), that are separated by a multiplicative ratio: (z/x)^(1/(y-1)). Constraints are: x,z > 0, y > 1, z-x >= y-1. For eg., if logfreq3(10,25,1000) is used in a variable by the *fix print* command, then the interval between 10 and 1000 is divided into 24 parts with a multiplicative separation of ~1.21, and it will generate the following sequence of output timesteps:

```
10, 13, 15, 18, 22, 27, 32,...384, 465, 563, 682, 826, 1000
```

The stride(x,y,z) function uses the current timestep to generate a new timestep. X,y >= 0 and z > 0 and x <= y are required. The generated timesteps increase in increments of z, from x to y, i.e. it generates the sequence x,x+z,x+2z,...,y. If y-x is not a multiple of z, then similar to the way a for loop operates, the last value will be one that does not exceed y. For any current timestep, the next timestep in the sequence is returned. Thus if stride(1000,2000,100) is used in a variable by the *dump_modify every* command, it will generate the sequence of output timesteps:

```
1000,1100,1200, ... ,1900,2000
```

The stride2(x,y,z,a,b,c) function is similar to the stride() function except it generates two sets of strided timesteps, one at a coarser level and one at a finer level. Thus it is useful for debugging, e.g. to produce output every timestep at the point in simulation when a problem occurs. X,y >= 0 and z > 0 and x <= y are required, as are a,b >= 0 and c > 0 and a < b. Also, a >= x and b <= y are required so that the second stride is inside the first. The generated timesteps increase in increments of z, starting at x, until a is reached. At that point the timestep increases in increments of c, from a to b, then after b, increments by z are resumed until y is reached. For any current timestep, the next timestep in the sequence is returned. Thus if stride2(1000,2000,100,1350,1360,1) is used in a variable by the *dump_modify every* command, it will generate the sequence of output timesteps:

```
1000,1100,1200,1300,1350,1351,1352, ... 1359,1360,1400,1500, ... ,2000
```

The vdisplace(x,y) function takes 2 arguments: x = value0 and y = velocity, and uses the elapsed time to change the value by a linear displacement due to the applied velocity over the course of a run, according to this formula:

```
value = value0 + velocity*(timestep-startstep)*dt
```

where dt = the timestep size.

The run begins on startstep. Startstep can span multiple runs, using the *start* keyword of the *run* command. See the *run* command for details of how to do this. Note that the *thermo_style* keyword elaplong = timestep-startstep.

The swiggle(x,y,z) and cwiggle(x,y,z) functions each take 3 arguments: x = value0, y = amplitude, z = period. They use the elapsed time to oscillate the value by a sin() or cos() function over the course of a run, according to one of these formulas, where omega = 2 PI / period:

```
value = value0 + Amplitude * sin(omega*(timestep-startstep)*dt)
value = value0 + Amplitude * (1 - cos(omega*(timestep-startstep)*dt))
```

where dt = the timestep size.

The run begins on startstep. Startstep can span multiple runs, using the *start* keyword of the *run* command. See the *run* command for details of how to do this. Note that the *thermo_style* keyword elaplong = timestep-startstep.

Group and Region Functions

Group functions are specified as keywords followed by one or two parenthesized arguments. The first argument *ID* is the group-ID. The *dim* argument, if it exists, is *x* or *y* or *z*. The *dir* argument, if it exists, is *xmin*, *xmax*, *ymin*, *ymax*, *zmin*, or *zmax*. The *dimdim* argument, if it exists, is *xx* or *yy* or *zz* or *xy* or *yz* or *xz*.

The group function count() is the number of atoms in the group. The group functions mass() and charge() are the total mass and charge of the group. Xcm() and vcm() return components of the position and velocity of the center of mass of the group. Fcm() returns a component of the total force on the group of atoms. Bound() returns the min/max of a particular coordinate for all atoms in the group. Gyration() computes the radius-of-gyration of the group of atoms. See the *compute gyration* command for a definition of the formula. Angmom() returns components of the angular momentum of the group of atoms around its center of mass. Torque() returns components of the torque on the group of atoms around its center of mass, based on current forces on the atoms. Inertia() returns one of 6 components of the symmetric inertia tensor of the group of atoms around its center of mass, ordered as Ixx,Iyy,Izz,Ixy,Iyz,Ixz. Omega() returns components of the angular velocity of the group of atoms around its center of mass.

Region functions are specified exactly the same way as group functions except they take an extra final argument *IDR* which is the region ID. The function is computed for all atoms that are in both the group and the region. If the group is "all", then the only criteria for atom inclusion is that it be in the region.

Special Functions

Special functions take specific kinds of arguments, meaning their arguments cannot be formulas themselves.

The sum(x), min(x), max(x), ave(x), trap(x), and slope(x) functions each take 1 argument which is of the form "c_ID" or "c_ID[N]" or "f_ID" or "f_ID[N]" or "v_name". The first two are computes and the second two are fixes; the ID in the reference should be replaced by the ID of a compute or fix defined elsewhere in the input script. The compute or fix must produce either a global vector or array. If it produces a global vector, then the notation without "[N]" should be used. If it produces a global array, then the notation with "[N]" should be used, when N is an integer, to specify which column of the global array is being referenced. The last form of argument "v_name" is for a vector-style variable where "name" is replaced by the name of the variable.

These functions operate on a global vector of inputs and reduce it to a single scalar value. This is analogous to the operation of the *compute reduce* command, which performs similar operations on per-atom and local vectors.

The sum() function calculates the sum of all the vector elements. The min() and max() functions find the minimum and maximum element respectively. The ave() function is the same as sum() except that it divides the result by the length of the vector.

The trap() function is the same as sum() except the first and last elements are multiplied by a weighting factor of 1/2 when performing the sum. This effectively implements an integration via the trapezoidal rule on the global vector of data. I.e. consider a set of points, equally spaced by 1 in their x coordinate: (1,V1), (2,V2), . . . , (N,VN), where the Vi are the values in the global vector of length N. The integral from 1 to N of these points is trap(). When appropriately normalized by the timestep size, this function is useful for calculating integrals of time-series data, like that generated by the *fix ave/correlate* command.

The slope() function uses linear regression to fit a line to the set of points, equally spaced by 1 in their x coordinate: (1,V1), (2,V2), . . . , (N,VN), where the Vi are the values in the global vector of length N. The returned value is the slope of the line. If the line has a single point or is vertical, it returns 1.0e20.

The gmask(x) function takes 1 argument which is a group ID. It can only be used in atom-style variables. It returns a 1 for atoms that are in the group, and a 0 for atoms that are not.

The rmask(x) function takes 1 argument which is a region ID. It can only be used in atom-style variables. It returns a 1 for atoms that are in the geometric region, and a 0 for atoms that are not.

The grmask(x,y) function takes 2 arguments. The first is a group ID, and the second is a region ID. It can only be used in atom-style variables. It returns a 1 for atoms that are in both the group and region, and a 0 for atoms that are not in both.

The next(x) function takes 1 argument which is a variable ID (not "v_foo", just "foo"). It must be for a file-style or atomfile-style variable. Each time the next() function is invoked (i.e. each time the equal-style or atom-style variable is evaluated), the following steps occur.

For file-style variables, the current string value stored by the file-style variable is converted to a numeric value and returned by the function. And the next string value in the file is read and stored. Note that if the line previously read from the file was not a numeric string, then it will typically evaluate to 0.0, which is likely not what you want.

For atomfile-style variables, the current per-atom values stored by the atomfile-style variable are returned by the function. And the next set of per-atom values in the file is read and stored.

Since file-style and atomfile-style variables read and store the first line of the file or first set of per-atoms values when they are defined in the input script, these are the value(s) that will be returned the first time the next() function is invoked. If next() is invoked more times than there are lines or sets of lines in the file, the variable is deleted, similar to how the *next* command operates.

Feature Functions

Feature functions allow to probe the running LAMMPS executable for whether specific features are either active, defined, or available. The functions take two arguments, a *category* and a corresponding *argument*. The arguments are strings thus cannot be formulas themselves (only $-style immediate variable expansion is possible). Return value is either 1.0 or 0.0 depending on whether the function evaluates to true or false, respectively.

The *is_active()* function allows to query for active settings which are grouped by categories. Currently supported categories and arguments are:

- *package* (argument = *gpu* or *intel* or *kokkos* or *omp*)
- *newton* (argument = *pair* or *bond* or *any*)
- *pair* (argument = *single* or *respa* or *manybody* or *tail* or *shift*)
- *comm_style* (argument = *brick* or *tiled*)
- *min_style* (argument = any of the compiled in minimizer styles)
- *run_style* (argument = any of the compiled in run styles)
- *atom_style* (argument = any of the compiled in atom styles)
- *pair_style* (argument = any of the compiled in pair styles)
- *bond_style* (argument = any of the compiled in bond styles)
- *angle_style* (argument = any of the compiled in angle styles)
- *dihedral_style* (argument = any of the compiled in dihedral styles)
- *improper_style* (argument = any of the compiled in improper styles)
- *kspace_style* (argument = any of the compiled in kspace styles)

Most of the settings are self-explanatory, the *single* argument in the *pair* category allows to check whether a pair style supports a Pair::single() function as needed by compute group/group and others features or LAMMPS, *respa* allows to check whether the inner/middle/outer mode of r-RESPA is supported. In the various style categories, the checking is also done using suffix flags, if available and enabled.

Example 1: disable use of suffix for pppm when using GPU package (i.e. run it on the CPU concurrently to running the pair style on the GPU), but do use the suffix otherwise (e.g. with USER-OMP).

```
pair_style lj/cut/coul/long 14.0
if $(is_active(package,gpu)) then "suffix off"
kspace_style pppm
```

Example 2: use r-RESPA with inner/outer cutoff, if supported by pair style, otherwise fall back to using pair and reducing the outer time step

```
timestep $(2.0*(1.0+2.0*is_active(pair,respa))
if $(is_active(pair,respa)) then "run_style respa 4 3 2 2  improper 1 inner␣
↪2 5.5 7.0 outer 3 kspace 4" else "run_style respa 3 3 2  improper 1 pair 2␣
↪kspace 3"
```

The *is_defined()* function allows to query categories like *compute*, *dump*, *fix*, *group*, *region*, and *variable* whether an entry with the provided name or id is defined.

The *is_available(category,name)* function allows to query whether a specific optional feature is available, i.e. compiled in. This currently works for the following categories: *command*, *compute*, *fix*, *pair_style* and *feature*. For all categories except *command* and *feature* also appending active suffixes is tried before reporting failure.

The *feature* category is used to check the availability of compiled in features such as GZIP support, PNG support, JPEG support, FFMPEG support, and C++ exceptions for error handling. Corresponding values for name are *gzip*, *png*, *jpeg*, *ffmpeg* and *exceptions*.

This enables writing input scripts which only dump using a given format if the compiled binary supports it.

```
if "$(is_available(feature,png))" then "print 'PNG supported'" else "print 'PNG not␣
↪supported'"

if "$(is_available(feature,ffmpeg)" then "dump 3 all movie 25 movie.mp4 type type␣
↪zoom 1.6 adiam 1.0"
```

Atom Values and Vectors

Atom values take an integer argument I from 1 to N, where I is the atom-ID, e.g. x[243], which means use the x coordinate of the atom with ID = 243. Or they can take a variable name, specified as v_name, where name is the name of the variable, like x[v_myIndex]. The variable can be of any style except *vector* or *atom* or *atomfile* variables. The variable is evaluated and the result is expected to be numeric and is cast to an integer (i.e. 3.4 becomes 3), to use an index, which must be a value from 1 to N. Note that a "formula" cannot be used as the argument between the brackets, e.g. x[243+10] or x[v_myIndex+1] are not allowed. To do this a single variable can be defined that contains the needed formula.

Note that the 0 < atom-ID <= N, where N is the largest atom ID in the system. If an ID is specified for an atom that does not currently exist, then the generated value is 0.0.

Atom vectors generate one value per atom, so that a reference like "vx" means the x-component of each atom's velocity will be used when evaluating the variable.

The meaning of the different atom values and vectors is mostly self-explanatory. *Mol* refers to the molecule ID of an atom, and is only defined if an *atom_style* is being used that defines molecule IDs.

Note that many other atom attributes can be used as inputs to a variable by using the *compute property/atom* command and then specifying a quantity from that compute.

Compute References

Compute references access quantities calculated by a *compute*. The ID in the reference should be replaced by the ID of a compute defined elsewhere in the input script. As discussed in the doc page for the *compute* command, computes can produce global, per-atom, or local values. Only global and per-atom values can be used in a variable. Computes can also produce a scalar, vector, or array.

An equal-style variable can only use scalar values, which means a global scalar, or an element of a global or per-atom vector or array. A vector-style variable can use scalar values or a global vector of values, or a column of a global array of values. Atom-style variables can use global scalar values. They can also use per-atom vector values, or a column of a per-atom array. See the doc pages for individual computes to see what kind of values they produce.

Examples of different kinds of compute references are as follows. There is typically no ambiguity (see exception below) as to what a reference means, since computes only produce either global or per-atom quantities, never both.

c_ID	global scalar, or per-atom vector
c_ID[I]	Ith element of global vector, or atom I's value in per-atom vector, or Ith column from per-atom array
c_ID[I][J]	I,J element of global array, or atom I's Jth value in per-atom array

For I and J indices, integers can be specified or a variable name, specified as v_name, where name is the name of the variable. The rules for this syntax are the same as for the "Atom Values and Vectors" discussion above.

One source of ambiguity for compute references is when a vector-style variable refers to a compute that produces both a global scalar and a global vector. Consider a compute with ID "foo" that does this, referenced as follows by variable "a", where "myVec" is another vector-style variable:

```
variable a vector c_foo*v_myVec
```

The reference "c_foo" could refer to either the global scalar or global vector produced by compute "foo". In this case, "c_foo" will always refer to the global scalar, and "C_foo" can be used to reference the global vector. Similarly if the compute produces both a global vector and global array, then "c_foo[I]" will always refer to an element of the global vector, and "C_foo[I]" can be used to reference the Ith column of the global array.

Note that if a variable containing a compute is evaluated directly in an input script (not during a run), then the values accessed by the compute must be current. See the discussion below about "Variable Accuracy".

Fix References

Fix references access quantities calculated by a *fix*. The ID in the reference should be replaced by the ID of a fix defined elsewhere in the input script. As discussed in the doc page for the *fix* command, fixes can produce global, per-atom, or local values. Only global and per-atom values can be used in a variable. Fixes can also produce a scalar, vector, or array. An equal-style variable can only use scalar values, which means a global scalar, or an element of a global or per-atom vector or array. Atom-style variables can use the same scalar values. They can also use per-atom vector values. A vector value can be a per-atom vector itself, or a column of an per-atom array. See the doc pages for individual fixes to see what kind of values they produce.

The different kinds of fix references are exactly the same as the compute references listed in the above table, where "c_" is replaced by "f_". Again, there is typically no ambiguity (see exception below) as to what a reference means, since fixes only produce either global or per-atom quantities, never both.

f_ID	global scalar, or per-atom vector
f_ID[I]	Ith element of global vector, or atom I's value in per-atom vector, or Ith column from per-atom array
f_ID[I][J]	I,J element of global array, or atom I's Jth value in per-atom array

For I and J indices, integers can be specified or a variable name, specified as v_name, where name is the name of the variable. The rules for this syntax are the same as for the "Atom Values and Vectors" discussion above.

One source of ambiguity for fix references is the same ambiguity discussed for compute references above. Namely when a vector-style variable refers to a fix that produces both a global scalar and a global vector. The solution is the same as for compute references. For a fix with ID "foo", "f_foo" will always refer to the global scalar, and "F_foo" can be used to reference the global vector. And similarly for distinguishing between a fix's global vector versus global array with "f_foo[I]" versus "F_foo[I]".

Note that if a variable containing a fix is evaluated directly in an input script (not during a run), then the values accessed by the fix should be current. See the discussion below about "Variable Accuracy".

Note that some fixes only generate quantities on certain timesteps. If a variable attempts to access the fix on non-allowed timesteps, an error is generated. For example, the *fix ave/time* command may only generate averaged quantities every 100 steps. See the doc pages for individual fix commands for details.

Variable References

Variable references access quantities stored or calculated by other variables, which will cause those variables to be evaluated. The name in the reference should be replaced by the name of a variable defined elsewhere in the input script.

As discussed on this doc page, equal-style variables generate a single global numeric value, vector-style variables generate a vector of global numeric values, and atom-style and atomfile-style variables generate a per-atom vector of numeric values. All other variables store one or more strings.

The formula for an equal-style variable can use any style of variable including a vector_style or atom-style or atomfile-style. For these 3 styles, a subscript must be used to access a single value from the vector-, atom-, or atomfile-style variable. If a string-storing variable is used, the string is converted to a numeric value. Note that this will typically produce a 0.0 if the string is not a numeric string, which is likely not what you want.

The formula for a vector-style variable can use any style of variable, including atom-style or atomfile-style variables. For these 2 styles, a subscript must be used to access a single value from the atom-, or atomfile-style variable.

The formula for an atom-style variable can use any style of variable, including other atom-style or atomfile-style variables. If it uses a vector-style variable, a subscript must be used to access a single value from the vector-style variable.

Examples of different kinds of variable references are as follows. There is no ambiguity as to what a reference means, since variables produce only a global scalar or global vector or per-atom vector.

v_name	global scalar from equal-style variable
v_name	global vector from vector-style variable
v_name	per-atom vector from atom-style or atomfile-style variable
v_name[I]	Ith element of a global vector from vector-style variable
v_name[I]	value of atom with ID = I from atom-style or atomfile-style variable

For the I index, an integer can be specified or a variable name, specified as v_name, where name is the name of the variable. The rules for this syntax are the same as for the "Atom Values and Vectors" discussion above.

Immediate Evaluation of Variables:

If you want an equal-style variable to be evaluated immediately, it may be the case that you do not need to define a variable at all. See the *Commands parse* doc page for info on how to use "immediate" variables in an input script, specified as $(formula) with parenthesis, where the formula has the same syntax as equal-style variables described on this page. This effectively evaluates a formula immediately without using the variable command to define a named variable.

More generally, there is a difference between referencing a variable with a leading $ sign (e.g. $x or ${abc}) versus with a leading "v_" (e.g. v_x or v_abc). The former can be used in any input script command, including a variable command. The input script parser evaluates the reference variable immediately and substitutes its value into the command. As explained on the *Commands parse* doc page, you can also use un-named "immediate" variables for this purpose. For example, a string like this $((xlo+xhi)/2+sqrt(v_area)) in an input script command evaluates the string between the parenthesis as an equal-style variable formula.

Referencing a variable with a leading "v_" is an optional or required kind of argument for some commands (e.g. the *fix ave/chunk* or *dump custom* or *thermo_style* commands) if you wish it to evaluate a variable periodically during a run. It can also be used in a variable formula if you wish to reference a second variable. The second variable will be evaluated whenever the first variable is evaluated.

As an example, suppose you use this command in your input script to define the variable "v" as

```
variable v equal vol
```

before a run where the simulation box size changes. You might think this will assign the initial volume to the variable "v". That is not the case. Rather it assigns a formula which evaluates the volume (using the thermo_style keyword "vol") to the variable "v". If you use the variable "v" in some other command like *fix ave/time* then the current volume of the box will be evaluated continuously during the run.

If you want to store the initial volume of the system, you can do it this way:

```
variable v equal vol
variable v0 equal $v
```

The second command will force "v" to be evaluated (yielding the initial volume) and assign that value to the variable "v0". Thus the command

```
thermo_style custom step v_v v_v0
```

would print out both the current and initial volume periodically during the run.

Note that it is a mistake to enclose a variable formula in double quotes if it contains variables preceded by $ signs. For example,

```
variable vratio equal "${vfinal}/${v0}"
```

This is because the quotes prevent variable substitution (explained on the *Commands parse* doc page), and thus an error will occur when the formula for "vratio" is evaluated later.

Variable Accuracy:

Obviously, LAMMPS attempts to evaluate variables containing formulas (*equal* and *atom* style variables) accurately whenever the evaluation is performed. Depending on what is included in the formula, this may require invoking a *compute*, either directly or indirectly via a thermo keyword, or accessing a value previously calculated by a compute, or accessing a value calculated and stored by a *fix*. If the compute is one that calculates the pressure or energy of the system, then these quantities need to be tallied during the evaluation of the interatomic potentials (pair, bond, etc) on timesteps that the variable will need the values.

LAMMPS keeps track of all of this during a *run* or *energy minimization*. An error will be generated if you attempt to evaluate a variable on timesteps when it cannot produce accurate values. For example, if a *thermo_style custom* command prints a variable which accesses values stored by a *fix ave/time* command and the timesteps on which thermo output is generated are not multiples of the averaging frequency used in the fix command, then an error will occur.

An input script can also request variables be evaluated before or after or in between runs, e.g. by including them in a *print* command. In this case, if a compute is needed to evaluate a variable (either directly or indirectly), LAMMPS will not invoke the compute, but it will use a value previously calculated by the compute, and can do this only if it was invoked on the current timestep. Fixes will always provide a quantity needed by a variable, but the quantity may or may not be current. This leads to one of three kinds of behavior:

(1) The variable may be evaluated accurately. If it contains references to a compute or fix, and these values were calculated on the last timestep of a preceding run, then they will be accessed and used by the variable and the result will be accurate.

(2) LAMMPS may not be able to evaluate the variable and will generate an error message stating so. For example, if the variable requires a quantity from a *compute* that has not been invoked on the current timestep, LAMMPS will generate an error. This means, for example, that such a variable cannot be evaluated before the first run has occurred. Likewise, in between runs, a variable containing a compute cannot be evaluated unless the compute was invoked on the last timestep of the preceding run, e.g. by thermodynamic output.

One way to get around this problem is to perform a 0-timestep run before using the variable. For example, these commands

```
variable t equal temp
print "Initial temperature = $t"
run 1000
```

will generate an error if the run is the first run specified in the input script, because generating a value for the "t" variable requires a compute for calculating the temperature to be invoked.

However, this sequence of commands would be fine:

```
run 0
variable t equal temp
print "Initial temperature = $t"
run 1000
```

The 0-timestep run initializes and invokes various computes, including the one for temperature, so that the value it stores is current and can be accessed by the variable "t" after the run has completed. Note that a 0-timestep run does not alter the state of the system, so it does not change the input state for the 1000-timestep run that follows. Also note that the 0-timestep run must actually use and invoke the compute in question (e.g. via *thermo* or *dump* output) in order for it to enable the compute to be used in a variable after the run. Thus if you are trying to print a variable that uses a compute you have defined, you can insure it is invoked on the last timestep of the preceding run by including it in thermodynamic output.

Unlike computes, *fixes* will never generate an error if their values are accessed by a variable in between runs. They always return some value to the variable. However, the value may not be what you expect if the fix has not yet calculated the quantity of interest or it is not current. For example, the *fix indent* command stores the force on the indenter. But this is not computed until a run is performed. Thus if a variable attempts to print this value before the first run, zeroes will be output. Again, performing a 0-timestep run before printing the variable has the desired effect.

(3) The variable may be evaluated incorrectly and LAMMPS may have no way to detect this has occurred. Consider the following sequence of commands:

```
pair_coeff 1 1 1.0 1.0
run 1000
pair_coeff 1 1 1.5 1.0
```

(continues on next page)

(continued from previous page)

```
variable e equal pe
print "Final potential energy = $e"
```

The first run is performed using one setting for the pairwise potential defined by the *pair_style* and *pair_coeff* commands. The potential energy is evaluated on the final timestep and stored by the *compute pe* compute (this is done by the *thermo_style* command). Then a pair coefficient is changed, altering the potential energy of the system. When the potential energy is printed via the "e" variable, LAMMPS will use the potential energy value stored by the *compute pe* compute, thinking it is current. There are many other commands which could alter the state of the system between runs, causing a variable to evaluate incorrectly.

The solution to this issue is the same as for case (2) above, namely perform a 0-timestep run before the variable is evaluated to insure the system is up-to-date. For example, this sequence of commands would print a potential energy that reflected the changed pairwise coefficient:

```
pair_coeff 1 1 1.0 1.0
run 1000
pair_coeff 1 1 1.5 1.0
run 0
variable e equal pe
print "Final potential energy = $e"
```

15.129.4 Restrictions

Indexing any formula element by global atom ID, such as an atom value, requires the *atom style* to use a global mapping in order to look up the vector indices. By default, only atom styles with molecular information create global maps. The *atom_modify map* command can override the default, e.g. for atomic-style atom styles.

All *universe*- and *uloop*-style variables defined in an input script must have the same number of values.

15.129.5 Related commands

next, *jump*, *include*, *temper*, *fix print*, *print*

Default: none

15.130 velocity command

15.130.1 Syntax

```
velocity group-ID style args keyword value ...
```

- group-ID = ID of group of atoms whose velocity will be changed
- style = *create* or *set* or *scale* or *ramp* or *zero*

```
create args = temp seed
  temp = temperature value (temperature units)
  seed = random # seed (positive integer)
set args = vx vy vz
  vx,vy,vz = velocity value or NULL (velocity units)
```

```
  any of vx,vy,vz van be a variable (see below)
scale arg = temp
  temp = temperature value (temperature units)
ramp args = vdim vlo vhi dim clo chi
  vdim = vx or vy or vz
  vlo,vhi = lower and upper velocity value (velocity units)
  dim = x or y or z
  clo,chi = lower and upper coordinate bound (distance units)
zero arg = linear or angular
  linear = zero the linear momentum
  angular = zero the angular momentum
```

- zero or more keyword/value pairs may be appended
- keyword = *dist* or *sum* or *mom* or *rot* or *temp* or *bias* or *loop* or *units*

```
dist value = uniform or gaussian
sum value = no or yes
mom value = no or yes
rot value = no or yes
temp value = temperature compute ID
bias value = no or yes
loop value = all or local or geom
rigid value = fix-ID
  fix-ID = ID of rigid body fix
units value = box or lattice
```

15.130.2 Examples

```
velocity all create 300.0 4928459 rot yes dist gaussian
velocity border set NULL 4.0 v_vz sum yes units box
velocity flow scale 300.0
velocity flow ramp vx 0.0 5.0 y 5 25 temp mytemp
velocity all zero linear
```

15.130.3 Description

Set or change the velocities of a group of atoms in one of several styles. For each style, there are required arguments and optional keyword/value parameters. Not all options are used by each style. Each option has a default as listed below.

The *create* style generates an ensemble of velocities using a random number generator with the specified seed at the specified temperature.

The *set* style sets the velocities of all atoms in the group to the specified values. If any component is specified as NULL, then it is not set. Any of the vx,vy,vz velocity components can be specified as an equal-style or atom-style *variable*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated, and its value used to determine the velocity component. Note that if a variable is used, the velocity it calculates must be in box units, not lattice units; see the discussion of the *units* keyword below.

Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters or other parameters.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent velocity field.

The *scale* style computes the current temperature of the group of atoms and then rescales the velocities to the specified temperature.

The *ramp* style is similar to that used by the *compute temp/ramp* command. Velocities ramped uniformly from vlo to vhi are applied to dimension vx, or vy, or vz. The value assigned to a particular atom depends on its relative coordinate value (in dim) from clo to chi. For the example above, an atom with y-coordinate of 10 (1/4 of the way from 5 to 25), would be assigned a x-velocity of 1.25 (1/4 of the way from 0.0 to 5.0). Atoms outside the coordinate bounds (less than 5 or greater than 25 in this case), are assigned velocities equal to vlo or vhi (0.0 or 5.0 in this case).

The *zero* style adjusts the velocities of the group of atoms so that the aggregate linear or angular momentum is zero. No other changes are made to the velocities of the atoms. If the *rigid* option is specified (see below), then the zeroing is performed on individual rigid bodies, as defined by the *fix rigid or fix rigid/small* commands. In other words, zero linear will set the linear momentum of each rigid body to zero, and zero angular will set the angular momentum of each rigid body to zero. This is done by adjusting the velocities of the atoms in each rigid body.

All temperatures specified in the velocity command are in temperature units; see the *units* command. The units of velocities and coordinates depend on whether the *units* keyword is set to *box* or *lattice*, as discussed below.

For all styles, no atoms are assigned z-component velocities if the simulation is 2d; see the *dimension* command.

The keyword/value options are used in the following ways by the various styles.

The *dist* keyword is used by *create*. The ensemble of generated velocities can be a *uniform* distribution from some minimum to maximum value, scaled to produce the requested temperature. Or it can be a *gaussian* distribution with a mean of 0.0 and a sigma scaled to produce the requested temperature.

The *sum* keyword is used by all styles, except *zero*. The new velocities will be added to the existing ones if sum = yes, or will replace them if sum = no.

The *mom* and *rot* keywords are used by *create*. If mom = yes, the linear momentum of the newly created ensemble of velocities is zeroed; if rot = yes, the angular momentum is zeroed.

If specified, the *temp* keyword is used by *create* and *scale* to specify a *compute* that calculates temperature in a desired way, e.g. by first subtracting out a velocity bias, as discussed on the *Howto thermostat* doc page. If this keyword is not specified, *create* and *scale* calculate temperature using a compute that is defined internally as follows:

```
compute velocity_temp group-ID temp
```

where group-ID is the same ID used in the velocity command. i.e. the group of atoms whose velocity is being altered. This compute is deleted when the velocity command is finished. See the *compute temp* command for details. If the calculated temperature should have degrees-of-freedom removed due to fix constraints (e.g. SHAKE or rigid-body constraints), then the appropriate fix command must be specified before the velocity command is issued.

The *bias* keyword with a *yes* setting is used by *create* and *scale*, but only if the *temp* keyword is also used to specify a *compute* that calculates temperature in a desired way. If the temperature compute also calculates a velocity bias, the bias is subtracted from atom velocities before the *create* and *scale* operations are performed. After the operations, the bias is added back to the atom velocities. See the *Howto thermostat* doc page for more discussion of temperature computes with biases. Note that the velocity bias is only applied to atoms in the temperature compute specified with the *temp* keyword.

As an example, assume atoms are currently streaming in a flow direction (which could be separately initialized with the *ramp* style), and you wish to initialize their thermal velocity to a desired temperature. In this context thermal velocity means the per-particle velocity that remains when the streaming velocity is subtracted. This can be done using the *create* style with the *temp* keyword specifying the ID of a *compute temp/ramp* or *compute temp/profile* command, and the *bias* keyword set to a *yes* value.

The *loop* keyword is used by *create* in the following ways.

If loop = all, then each processor loops over all atoms in the simulation to create velocities, but only stores velocities for atoms it owns. This can be a slow loop for a large simulation. If atoms were read from a data file, the velocity assigned to a particular atom will be the same, independent of how many processors are being used. This will not be the case if atoms were created using the *create_atoms* command, since atom IDs will likely be assigned to atoms differently.

If loop = local, then each processor loops over only its atoms to produce velocities. The random number seed is adjusted to give a different set of velocities on each processor. This is a fast loop, but the velocity assigned to a particular atom will depend on which processor owns it. Thus the results will always be different when a simulation is run on a different number of processors.

If loop = geom, then each processor loops over only its atoms. For each atom a unique random number seed is created, based on the atom's xyz coordinates. A velocity is generated using that seed. This is a fast loop and the velocity assigned to a particular atom will be the same, independent of how many processors are used. However, the set of generated velocities may be more correlated than if the *all* or *local* keywords are used.

Note that the *loop geom* keyword will not necessarily assign identical velocities for two simulations run on different machines. This is because the computations based on xyz coordinates are sensitive to tiny differences in the double-precision value for a coordinate as stored on a particular machine.

The *rigid* keyword only has meaning when used with the *zero* style. It allows specification of a fix-ID for one of the *rigid-body fix* variants which defines a set of rigid bodies. The zeroing of linear or angular momentum is then performed for each rigid body defined by the fix, as described above.

The *units* keyword is used by *set* and *ramp*. If units = box, the velocities and coordinates specified in the velocity command are in the standard units described by the *units* command (e.g. Angstroms/fmsec for real units). If units = lattice, velocities are in units of lattice spacings per time (e.g. spacings/fmsec) and coordinates are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacing.

15.130.4 Restrictions

Assigning a temperature via the *create* style to a system with *rigid bodies* or *SHAKE constraints* may not have the desired outcome for two reasons. First, the velocity command can be invoked before all of the relevant fixes are created and initialized and the number of adjusted degrees of freedom (DOFs) is known. Thus it is not possible to compute the target temperature correctly. Second, the assigned velocities may be partially canceled when constraints are first enforced, leading to a different temperature than desired. A workaround for this is to perform a *run 0* command, which insures all DOFs are accounted for properly, and then rescale the temperature to the desired value before performing a simulation. For example:

```
velocity all create 300.0 12345
run 0                           # temperature may not be 300K
velocity all scale 300.0        # now it should be
```

15.130.5 Related commands

fix rigid, *fix shake*, *lattice*

15.130.6 Default

The keyword defaults are dist = uniform, sum = no, mom = yes, rot = no, bias = no, loop = all, and units = lattice. The temp and rigid keywords are not defined by default.

15.131 write_coeff command

15.131.1 Syntax

```
write_coeff file
```

- file = name of data file to write out

15.131.2 Examples

```
write_coeff polymer.coeff
```

15.131.3 Description

Write a text format file with the currently defined force field coefficients in a way, that it can be read by LAMMPS with the *include* command. In combination with the nocoeff option of *write_data* this can be used to move the Coeffs sections from a data file into a separate file.

Note: The write_coeff command is not yet fully implemented as some pair styles do not output their coefficient information. This means you will need to add/copy this information manually.

15.131.4 Restrictions

none

15.131.5 Related commands

read_data, *write_restart*, *write_data*

15.132 write_data command

15.132.1 Syntax

```
write_data file keyword value ...
```

- file = name of data file to write out
- zero or more keyword/value pairs may be appended
- keyword = *pair* or *nocoeff*

```
nocoeff = do not write out force field info
nofix = do not write out extra sections read by fixes
pair value = ii or ij
  ii = write one line of pair coefficient info per atom type
  ij = write one line of pair coefficient info per IJ atom type pair
```

15.132.2 Examples

```
write_data data.polymer
write_data data.*
```

15.132.3 Description

Write a data file in text format of the current state of the simulation. Data files can be read by the *read data* command to begin a simulation. The *read_data* command also describes their format.

Similar to *dump* files, the data filename can contain a "*" wild-card character. The "*" is replaced with the current timestep value.

Note: The write-data command is not yet fully implemented in two respects. First, most pair styles do not yet write their coefficient information into the data file. This means you will need to specify that information in your input script that reads the data file, via the *pair_coeff* command. Second, a few of the *atom styles* (body, ellipsoid, line, tri) that store auxiliary "bonus" information about aspherical particles, do not yet write the bonus info into the data file. Both these functionalities will be added to the write_data command later.

Because a data file is in text format, if you use a data file written out by this command to restart a simulation, the initial state of the new run will be slightly different than the final state of the old run (when the file was written) which was represented internally by LAMMPS in binary format. A new simulation which reads the data file will thus typically diverge from a simulation that continued in the original input script.

If you want to do more exact restarts, using binary files, see the *restart*, *write_restart*, and *read_restart* commands. You can also convert binary restart files to text data files, after a simulation has run, using the *-r command-line switch*.

Note: Only limited information about a simulation is stored in a data file. For example, no information about atom *groups* and *fixes* are stored. *Binary restart files* store more information.

Bond interactions (angle, etc) that have been turned off by the *fix shake* or *delete_bonds* command will be written to a data file as if they are turned on. This means they will need to be turned off again in a new run after the data file is read.

Bonds that are broken (e.g. by a bond-breaking potential) are not written to the data file. Thus these bonds will not exist when the data file is read.

The *nocoeff* keyword requests that no force field parameters should be written to the data file. This can be very helpful, if one wants to make significant changes to the force field or if the parameters are read in separately anyway, e.g. from an include file.

The *nofix* keyword requests that no extra sections read by fixes should be written to the data file (see the *fix* option of the *read_data* command for details). For example, this option excludes sections for user-created per-atom properties from *fix property/atom*.

The *pair* keyword lets you specify in what format the pair coefficient information is written into the data file. If the value is specified as *ii*, then one line per atom type is written, to specify the coefficients for each of the I=J interactions. This means that no cross-interactions for I != J will be specified in the data file and the pair style will apply its mixing rule, as documented on individual *pair_style* doc pages. Of course this behavior can be overridden in the input script after reading the data file, by specifying additional *pair_coeff* commands for any desired I,J pairs.

If the value is specified as *ij*, then one line of coefficients is written for all I,J pairs where I <= J. These coefficients will include any specific settings made in the input script up to that point. The presence of these I != J coefficients in the data file will effectively turn off the default mixing rule for the pair style. Again, the coefficient values in the data file can be overridden in the input script after reading the data file, by specifying additional *pair_coeff* commands for any desired I,J pairs.

15.132.4 Restrictions

This command requires inter-processor communication to migrate atoms before the data file is written. This means that your system must be ready to perform a simulation before using this command (force fields setup, atom masses initialized, etc).

15.132.5 Related commands

read_data, *write_restart*

15.132.6 Default

The option defaults are pair = ii.

15.133 write_dump command

15.133.1 Syntax

```
write_dump group-ID style file dump-args modify dump_modify-args
```

- group-ID = ID of the group of atoms to be dumped
- style = any of the supported *dump styles*
- file = name of file to write dump info to
- dump-args = any additional args needed for a particular *dump style*

- modify = all args after this keyword are passed to *dump_modify* (optional)
- dump-modify-args = args for *dump_modify* (optional)

15.133.2 Examples

```
write_dump all atom dump.atom
write_dump subgroup atom dump.run.bin
write_dump all custom dump.myforce.* id type x y vx fx
write_dump flow custom dump.%.myforce id type c_myF[3] v_ke modify sort id
write_dump all xyz system.xyz modify sort id element O H
write_dump all image snap*.jpg type type size 960 960 modify backcolor white
write_dump all image snap*.jpg element element &
   bond atom 0.3 shiny 0.1 ssao yes 6345 0.2 size 1600 1600  &
   modify backcolor white element C C O H N C C C O H H S O H
```

15.133.3 Description

Dump a single snapshot of atom quantities to one or more files for the current state of the system. This is a one-time immediate operation, in contrast to the *dump* command which will will set up a dump style to write out snapshots periodically during a running simulation.

The syntax for this command is mostly identical to that of the *dump* and *dump_modify* commands as if they were concatenated together, with the following exceptions: There is no need for a dump ID or dump frequency and the keyword *modify* is added. The latter is so that the full range of *dump_modify* options can be specified for the single snapshot, just as they can be for multiple snapshots. The *modify* keyword separates the arguments that would normally be passed to the *dump* command from those that would be given the *dump_modify*. Both support optional arguments and thus LAMMPS needs to be able to cleanly separate the two sets of args.

Note that if the specified filename uses wildcard characters "*" or "%", as supported by the *dump* command, they will operate in the same fashion to create the new filename(s). Normally, *dump image* files require a filename with a "*" character for the timestep. That is not the case for the write_dump command; no wildcard "*" character is necessary.

15.133.4 Restrictions

All restrictions for the *dump* and *dump_modify* commands apply to this command as well, with the exception of the *dump image* filename not requiring a wildcard "*" character, as noted above.

Since dumps are normally written during a *run* or *energy minimization*, the simulation has to be ready to run before this command can be used. Similarly, if the dump requires information from a compute, fix, or variable, the information needs to have been calculated for the current timestep (e.g. by a prior run), else LAMMPS will generate an error message.

For example, it is not possible to dump per-atom energy with this command before a run has been performed, since no energies and forces have yet been calculated. See the *variable* doc page section on Variable Accuracy for more information on this topic.

15.133.5 Related commands

dump, *dump image*, *dump_modify*

15.133.6 Default

The defaults are listed on the doc pages for the *dump* and *dump image* and *dump_modify* commands.

15.134 write_restart command

15.134.1 Syntax

```
write_restart file keyword value ...
```

- file = name of file to write restart information to
- zero or more keyword/value pairs may be appended
- keyword = *fileper* or *nfile*

```
fileper arg = Np
  Np = write one file for every this many processors
nfile arg = Nf
  Nf = write this many files, one from each of Nf processors
```

15.134.2 Examples

```
write_restart restart.equil
write_restart restart.equil.mpiio
write_restart poly.%.* nfile 10
```

15.134.3 Description

Write a binary restart file of the current state of the simulation.

During a long simulation, the *restart* command is typically used to output restart files periodically. The write_restart command is useful after a minimization or whenever you wish to write out a single current restart file.

Similar to *dump* files, the restart filename can contain two wild-card characters. If a "*" appears in the filename, it is replaced with the current timestep value. If a "%" character appears in the filename, then one file is written by each processor and the "%" character is replaced with the processor ID from 0 to P-1. An additional file with the "%" replaced by "base" is also written, which contains global information. For example, the files written for filename restart.% would be restart.base, restart.0, restart.1, ... restart.P-1. This creates smaller files and can be a fast mode of output and subsequent input on parallel machines that support parallel I/O. The optional *fileper* and *nfile* keywords discussed below can alter the number of files written.

The restart file can also be written in parallel as one large binary file via the MPI-IO library, which is part of the MPI standard for versions 2.0 and above. Using MPI-IO requires two steps. First, build LAMMPS with its MPIIO package installed, e.g.

```
make yes-mpiio    # installs the MPIIO package
make mpi          # build LAMMPS for your platform
```

Second, use a restart filename which contains ".mpiio". Note that it does not have to end in ".mpiio", just contain those characters. Unlike MPI-IO dump files, a particular restart file must be both written and read using MPI-IO.

Restart files can be read by a *read_restart* command to restart a simulation from a particular state. Because the file is binary (to enable exact restarts), it may not be readable on another machine. In this case, you can use the *-r command-line switch* to convert a restart file to a data file.

Note: Although the purpose of restart files is to enable restarting a simulation from where it left off, not all information about a simulation is stored in the file. For example, the list of fixes that were specified during the initial run is not stored, which means the new input script must specify any fixes you want to use. Even when restart information is stored in the file, as it is for some fixes, commands may need to be re-specified in the new input script, in order to re-use that information. Details are usually given in the documentation of the respective command. Also, see the *read_restart* command for general information about what is stored in a restart file.

The optional *nfile* or *fileper* keywords can be used in conjunction with the "%" wildcard character in the specified restart file name. As explained above, the "%" character causes the restart file to be written in pieces, one piece for each of P processors. By default P = the number of processors the simulation is running on. The *nfile* or *fileper* keyword can be used to set P to a smaller value, which can be more efficient when running on a large number of processors.

The *nfile* keyword sets P to the specified Nf value. For example, if Nf = 4, and the simulation is running on 100 processors, 4 files will be written, by processors 0,25,50,75. Each will collect information from itself and the next 24 processors and write it to a restart file.

For the *fileper* keyword, the specified value of Np means write one file for every Np processors. For example, if Np = 4, every 4th processor (0,4,8,12,etc) will collect information from itself and the next 3 processors and write it to a restart file.

15.134.4 Restrictions

This command requires inter-processor communication to migrate atoms before the restart file is written. This means that your system must be ready to perform a simulation before using this command (force fields setup, atom masses initialized, etc).

To write and read restart files in parallel with MPI-IO, the MPIIO package must be installed.

15.134.5 Related commands

restart, *read_restart*, *write_data*

Default: none

CHAPTER

SIXTEEN

FIXES

16.1 fix adapt command

16.1.1 Syntax

```
fix ID group-ID adapt N attribute args ... keyword value ...
```

- ID, group-ID are documented in *fix* command
- adapt = style name of this fix command
- N = adapt simulation settings every this many timesteps
- one or more attribute/arg pairs may be appended
- attribute = *pair* or *kspace* or *atom*

```
pair args = pstyle pparam I J v_name
  pstyle = pair style name, e.g. lj/cut
  pparam = parameter to adapt over time
  I,J = type pair(s) to set parameter for
  v_name = variable with name that calculates value of pparam
bond args = bstyle bparam I v_name
  bstyle = bond style name, e.g. harmonic
  bparam = parameter to adapt over time
  I = type bond to set parameter for
  v_name = variable with name that calculates value of bparam
kspace arg = v_name
  v_name = variable with name that calculates scale factor on K-space␣
↪terms
atom args = aparam v_name
  aparam = parameter to adapt over time
  v_name = variable with name that calculates value of aparam
```

- zero or more keyword/value pairs may be appended
- keyword = *scale* or *reset*

```
scale value = no or yes
  no = the variable value is the new setting
  yes = the variable value multiplies the original setting
reset value = no or yes
  no = values will remain altered at the end of a run
  yes = reset altered values to their original values at the end of a run
```

16.1.2 Examples

```
fix 1 all adapt 1 pair soft a 1 1 v_prefactor
fix 1 all adapt 1 pair soft a 2* 3 v_prefactor
fix 1 all adapt 1 pair lj/cut epsilon * * v_scale1 coul/cut scale 3 3 v_
↪scale2 scale yes reset yes
fix 1 all adapt 10 atom diameter v_size

variable ramp_up equal "ramp(0.01,0.5)"
fix stretch all adapt 1 bond harmonic r0 1 v_ramp_up
```

16.1.3 Description

Change or adapt one or more specific simulation attributes or settings over time as a simulation runs. Pair potential and K-space and atom attributes which can be varied by this fix are discussed below. Many other fixes can also be used to time-vary simulation parameters, e.g. the "fix deform" command will change the simulation box size/shape and the "fix move" command will change atom positions and velocities in a prescribed manner. Also note that many commands allow variables as arguments for specific parameters, if described in that manner on their doc pages. An equal-style variable can calculate a time-dependent quantity, so this is another way to vary a simulation parameter over time.

If N is specified as 0, the specified attributes are only changed once, before the simulation begins. This is all that is needed if the associated variables are not time-dependent. If $N > 0$, then changes are made every N steps during the simulation, presumably with a variable that is time-dependent.

Depending on the value of the *reset* keyword, attributes changed by this fix will or will not be reset back to their original values at the end of a simulation. Even if *reset* is specified as *yes*, a restart file written during a simulation will contain the modified settings.

If the *scale* keyword is set to *no*, then the value the parameter is set to will be whatever the variable generates. If the *scale* keyword is set to *yes*, then the value of the altered parameter will be the initial value of that parameter multiplied by whatever the variable generates. I.e. the variable is now a "scale factor" applied in (presumably) a time-varying fashion to the parameter.

Note that whether scale is *no* or *yes*, internally, the parameters themselves are actually altered by this fix. Make sure you use the *reset yes* option if you want the parameters to be restored to their initial values after the run.

The *pair* keyword enables various parameters of potentials defined by the *pair_style* command to be changed, if the pair style supports it. Note that the *pair_style* and *pair_coeff* commands must be used in the usual manner to specify these parameters initially; the fix adapt command simply overrides the parameters.

The *pstyle* argument is the name of the pair style. If *pair_style hybrid or hybrid/overlay* is used, *pstyle* should be a sub-style name. If there are multiple sub-styles using the same pair style, then *pstyle* should be specified as "style:N" where N is which instance of the pair style you wish to adapt, e.g. the first, second, etc. For example, *pstyle* could be specified as "soft" or "lubricate" or "lj/cut:1" or "lj/cut:2". The *pparam* argument is the name of the parameter to change. This is the current list of pair styles and parameters that can be varied by this fix. See the doc pages for individual pair styles and their energy formulas for the meaning of these parameters:

born	a,b,c	type pairs
born/coul/long, born/coul/msm	coulombic_cutoff	type global
buck	a,c	type pairs
buck/coul/long, buck/coul/msm	coulombic_cutoff	type global
buck/mdf	a,c	type pairs

Continued on next page

Table 1 – continued from previous page

coul/cut	scale	type pairs
coul/cut/soft	lambda	type pairs
coul/debye	scale	type pairs
coul/dsf	coulombic_cutoff	type global
coul/long, coul/msm	coulombic_cutoff, scale	type pairs
coul/long/soft	scale, lambda, coulombic_cutoff	type pairs
eam, eam/alloy, eam/fs	scale	type pairs
gauss	a	type pairs
lennard/mdf	A,B	type pairs
lj/class2	epsilon,sigma	type pairs
lj/class2/coul/cut, lj/class2/coul/long	epsilon,sigma,coulombic_cutoff	type pairs
lj/cut	epsilon,sigma	type pairs
lj/cut/coul/cut, lj/cut/coul/long, lj/cut/coul/msm	epsilon,sigma,coulombic_cutoff	type pairs
lj/cut/coul/cut/soft, lj/cut/coul/long/soft	epsilon,sigma,lambda,coulombic_cutoff	type pairs
lj/cut/coul/dsf	cutoff	type global
lj/cut/tip4p/cut	epsilon,sigma,coulombic_cutoff	type pairs
lj/cut/soft	epsilon,sigma,lambda	type pairs
lj/expand	epsilon,sigma,delta	type pairs
lj/mdf	epsilon,sigma	type pairs
lj/sf/dipole/sf	epsilon,sigma,scale	type pairs
lubricate	mu	global
mie/cut	epsilon,sigma,gamma_repulsive,gamma_attractive	type pairs
morse, morse/smooth/linear	D0,R0,alpha	type pairs
morse/soft	D0,R0,alpha,lambda	type pairs
nm/cut	E0,R0,m,n	type pairs
nm/cut/coul/cut, nm/cut/coul/long	E0,R0,m,n,coulombic_cutoff	type pairs
reax/c	chi, eta, gamma	type global
spin/dmi	coulombic_cutoff	type global
spin/exchange	coulombic_cutoff	type global
spin/magelec	coulombic_cutoff	type global
spin/neel	coulombic_cutoff	type global
table	table_cutoff	type pairs
ufm	epsilon,sigma	type pairs
soft	a	type pairs

Note: It is easy to add new pairwise potentials and their parameters to this list. All it typically takes is adding an extract() method to the pair_*.cpp file associated with the potential.

Some parameters are global settings for the pair style, e.g. the viscosity setting "mu" for *pair_style lubricate*. Other parameters apply to atom type pairs within the pair style, e.g. the prefactor "a" for *pair_style soft*.

Note that for many of the potentials, the parameter that can be varied is effectively a prefactor on the entire energy expression for the potential, e.g. the lj/cut epsilon. The parameters listed as "scale" are exactly that, since the energy expression for the *coul/cut* potential (for example) has no labeled prefactor in its formula. To apply an effective prefactor to some potentials, multiple parameters need to be altered. For example, the *Buckingham potential* needs both the A and C terms altered together. To scale the Buckingham potential, you should thus list the pair style twice, once for A and once for C.

If a type pair parameter is specified, the *I* and *J* settings should be specified to indicate which type pairs to apply it to. If a global parameter is specified, the *I* and *J* settings still need to be specified, but are ignored.

Similar to the *pair_coeff command*, I and J can be specified in one of two ways. Explicit numeric values can be used for each, as in the 1st example above. I <= J is required. LAMMPS sets the coefficients for the symmetric J,I interaction to the same values.

A wild-card asterisk can be used in place of or in conjunction with the I,J arguments to set the coefficients for multiple pairs of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). Note that only type pairs with I <= J are considered; if asterisks imply type pairs where J < I, they are ignored.

IMPROTANT NOTE: If *pair_style hybrid or hybrid/overlay* is being used, then the *pstyle* will be a sub-style name. You must specify I,J arguments that correspond to type pair values defined (via the *pair_coeff* command) for that sub-style.

The *v_name* argument for keyword *pair* is the name of an *equal-style variable* which will be evaluated each time this fix is invoked to set the parameter to a new value. It should be specified as v_name, where name is the variable name. Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify parameters that change as a function of time or span consecutive runs in a continuous fashion. For the latter, see the *start* and *stop* keywords of the *run* command and the *elaplong* keyword of *thermo_style custom* for details.

For example, these commands would change the prefactor coefficient of the *pair_style soft* potential from 10.0 to 30.0 in a linear fashion over the course of a simulation:

```
variable prefactor equal ramp(10,30)
fix 1 all adapt 1 pair soft a * * v_prefactor
```

The *bond* keyword uses the specified variable to change the value of a bond coefficient over time, very similar to how the *pair* keyword operates. The only difference is that now a bond coefficient for a given bond type is adapted.

A wild-card asterisk can be used in place of or in conjunction with the bond type argument to set the coefficients for multiple bond types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

Currently *bond* does not support bond_style hybrid nor bond_style hybrid/overlay as bond styles. The only bonds that currently are working with fix_adapt are

gromos	k, r0	type bonds
harmonic	k,r0	type bonds

The *kspace* keyword used the specified variable as a scale factor on the energy, forces, virial calculated by whatever K-Space solver is defined by the *kspace_style* command. If the variable has a value of 1.0, then the solver is unaltered.

The *kspace* keyword works this way whether the *scale* keyword is set to *no* or *yes*.

The *atom* keyword enables various atom properties to be changed. The *aparam* argument is the name of the parameter to change. This is the current list of atom parameters that can be varied by this fix:

- charge = charge on particle
- diameter = diameter of particle

The *v_name* argument of the *atom* keyword is the name of an *equal-style variable* which will be evaluated each time this fix is invoked to set the parameter to a new value. It should be specified as v_name, where name is the variable name. See the discussion above describing the formulas associated with equal-style variables. The new value is assigned to the corresponding attribute for all atoms in the fix group.

Note: The *atom* keyword works this way whether the *scale* keyword is set to *no* or *yes*. I.e. the use of scale yes is not yet supported by the *atom* keyword.

If the atom parameter is *diameter* and per-atom density and per-atom mass are defined for particles (e.g. *atom_style granular*), then the mass of each particle is also changed when the diameter changes (density is assumed to stay constant).

For example, these commands would shrink the diameter of all granular particles in the "center" group from 1.0 to 0.1 in a linear fashion over the course of a 1000-step simulation:

```
variable size equal ramp(1.0,0.1)
fix 1 center adapt 10 atom diameter v_size
```

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

For *rRESPA time integration*, this fix changes parameters on the outermost rRESPA level.

16.1.4 Restrictions

none

16.1.5 Related commands

compute ti

16.1.6 Default

The option defaults are scale = no, reset = no.

16.2 fix adapt/fep command

16.2.1 Syntax

```
fix ID group-ID adapt/fep N attribute args ... keyword value ...
```

- ID, group-ID are documented in *fix* command
- adapt/fep = style name of this fix command
- N = adapt simulation settings every this many timesteps

- one or more attribute/arg pairs may be appended
- attribute = *pair* or *kspace* or *atom*

```
pair args = pstyle pparam I J v_name
  pstyle = pair style name, e.g. lj/cut
  pparam = parameter to adapt over time
  I,J = type pair(s) to set parameter for
  v_name = variable with name that calculates value of pparam
kspace arg = v_name
  v_name = variable with name that calculates scale factor on K-space␣
↪terms
atom args = aparam v_name
  aparam = parameter to adapt over time
  I = type(s) to set parameter for
  v_name = variable with name that calculates value of aparam
```

- zero or more keyword/value pairs may be appended
- keyword = *scale* or *reset* or *after*

```
scale value = no or yes
  no = the variable value is the new setting
  yes = the variable value multiplies the original setting
reset value = no or yes
  no = values will remain altered at the end of a run
  yes = reset altered values to their original values at the end
  of a run
after value = no or yes
  no = parameters are adapted at timestep N
  yes = parameters are adapted one timestep after N
```

16.2.2 Examples

```
fix 1 all adapt/fep 1 pair soft a 1 1 v_prefactor
fix 1 all adapt/fep 1 pair soft a 2* 3 v_prefactor
fix 1 all adapt/fep 1 pair lj/cut epsilon * * v_scale1 coul/cut scale 3 3 v_
↪scale2 scale yes reset yes
fix 1 all adapt/fep 10 atom diameter 1 v_size
```

16.2.3 Description

Change or adapt one or more specific simulation attributes or settings over time as a simulation runs.

This is an enhanced version of the *fix adapt* command with two differences,

- It is possible to modify the charges of chosen atom types only, instead of scaling all the charges in the system.
- There is a new option *after* for better compatibility with "fix ave/time".

This version is suited for free energy calculations using *compute ti* or *compute fep*.

If N is specified as 0, the specified attributes are only changed once, before the simulation begins. This is all that is needed if the associated variables are not time-dependent. If $N > 0$, then changes are made every N steps during the simulation, presumably with a variable that is time-dependent.

Depending on the value of the *reset* keyword, attributes changed by this fix will or will not be reset back to their original values at the end of a simulation. Even if *reset* is specified as *yes*, a restart file written during a simulation will contain the modified settings.

If the *scale* keyword is set to *no*, then the value the parameter is set to will be whatever the variable generates. If the *scale* keyword is set to *yes*, then the value of the altered parameter will be the initial value of that parameter multiplied by whatever the variable generates. I.e. the variable is now a "scale factor" applied in (presumably) a time-varying fashion to the parameter. Internally, the parameters themselves are actually altered; make sure you use the *reset yes* option if you want the parameters to be restored to their initial values after the run.

If the *after* keyword is set to *yes*, then the parameters are changed one timestep after the multiple of N. In this manner, if a fix such as "fix ave/time" is used to calculate averages at every N timesteps, all the contributions to the average will be obtained with the same values of the parameters.

The *pair* keyword enables various parameters of potentials defined by the *pair_style* command to be changed, if the pair style supports it. Note that the *pair_style* and *pair_coeff* commands must be used in the usual manner to specify these parameters initially; the fix adapt command simply overrides the parameters.

The *pstyle* argument is the name of the pair style. If *pair_style hybrid or hybrid/overlay* is used, *pstyle* should be a sub-style name. For example, *pstyle* could be specified as "soft" or "lubricate". The *pparam* argument is the name of the parameter to change. This is the current list of pair styles and parameters that can be varied by this fix. See the doc pages for individual pair styles and their energy formulas for the meaning of these parameters:

born	a,b,c	type pairs
buck	a,c	type pairs
buck/mdf	a,c	type pairs
coul/cut	scale	type pairs
coul/cut/soft	lambda	type pairs
coul/long, coul/msm	scale	type pairs
coul/long/soft	scale, lambda	type pairs
eam	scale	type pairs
gauss	a	type pairs
lennard/mdf	a,b	type pairs
lj/class2	epsilon,sigma	type pairs
lj/class2/coul/cut, lj/class2/coul/long	epsilon,sigma	type pairs
lj/cut	epsilon,sigma	type pairs
lj/cut/soft	epsilon,sigma,lambda	type pairs
lj/cut/coul/cut, lj/cut/coul/long, lj/cut/coul/msm	epsilon,sigma	type pairs
lj/cut/coul/cut/soft, lj/cut/coul/long/soft	epsilon,sigma,lambda	type pairs
lj/cut/tip4p/cut, lj/cut/tip4p/long	epsilon,sigma	type pairs
lj/cut/tip4p/long/soft	epsilon,sigma,lambda	type pairs
lj/expand	epsilon,sigma,delta	type pairs
lj/mdf	epsilon,sigma	type pairs
lj/sf/dipole/sf	epsilon,sigma,scale	type pairs
mie/cut	epsilon,sigma,gamR,gamA	type pairs
morse, morse/smooth/linear	d0,r0,alpha	type pairs
morse/soft	d0,r0,alpha,lambda	type pairs
nm/cut	e0,r0,nn,mm	type pairs
nm/cut/coul/cut, nm/cut/coul/long	e0,r0,nn,mm	type pairs
ufm	epsilon,sigma,scale	type pairs
soft	a	type pairs

Note: It is easy to add new potentials and their parameters to this list. All it typically takes is adding an extract() method to the pair_*.cpp file associated with the potential.

Note that for many of the potentials, the parameter that can be varied is effectively a prefactor on the entire energy expression for the potential, e.g. the lj/cut epsilon. The parameters listed as "scale" are exactly that, since the energy expression for the *coul/cut* potential (for example) has no labeled prefactor in its formula. To apply an effective prefactor to some potentials, multiple parameters need to be altered. For example, the *Buckingham potential* needs both the A and C terms altered together. To scale the Buckingham potential, you should thus list the pair style twice, once for A and once for C.

If a type pair parameter is specified, the *I* and *J* settings should be specified to indicate which type pairs to apply it to. If a global parameter is specified, the *I* and *J* settings still need to be specified, but are ignored.

Similar to the *pair_coeff command*, I and J can be specified in one of two ways. Explicit numeric values can be used for each, as in the 1st example above. I <= J is required. LAMMPS sets the coefficients for the symmetric J,I interaction to the same values.

A wild-card asterisk can be used in place of or in conjunction with the I,J arguments to set the coefficients for multiple pairs of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). Note that only type pairs with I <= J are considered; if asterisks imply type pairs where J < I, they are ignored.

IMPROTANT NOTE: If *pair_style hybrid or hybrid/overlay* is being used, then the *pstyle* will be a sub-style name. You must specify I,J arguments that correspond to type pair values defined (via the *pair_coeff* command) for that sub-style.

The *v_name* argument for keyword *pair* is the name of an *equal-style variable* which will be evaluated each time this fix is invoked to set the parameter to a new value. It should be specified as v_name, where name is the variable name. Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify parameters that change as a function of time or span consecutive runs in a continuous fashion. For the latter, see the *start* and *stop* keywords of the *run* command and the *elaplong* keyword of *thermo_style custom* for details.

For example, these commands would change the prefactor coefficient of the *pair_style soft* potential from 10.0 to 30.0 in a linear fashion over the course of a simulation:

```
variable prefactor equal ramp(10,30)
fix 1 all adapt 1 pair soft a * * v_prefactor
```

The *kspace* keyword used the specified variable as a scale factor on the energy, forces, virial calculated by whatever K-Space solver is defined by the *kspace_style* command. If the variable has a value of 1.0, then the solver is unaltered.

The *kspace* keyword works this way whether the *scale* keyword is set to *no* or *yes*.

The *atom* keyword enables various atom properties to be changed. The *aparam* argument is the name of the parameter to change. This is the current list of atom parameters that can be varied by this fix:

- charge = charge on particle
- diameter = diameter of particle

The *I* argument indicates which atom types are affected. A wild-card asterisk can be used in place of or in conjunction with the I argument to set the coefficients for multiple atom types.

The *v_name* argument of the *atom* keyword is the name of an *equal-style variable* which will be evaluated each time this fix is invoked to set the parameter to a new value. It should be specified as v_name, where name is the variable

name. See the discussion above describing the formulas associated with equal-style variables. The new value is assigned to the corresponding attribute for all atoms in the fix group.

If the atom parameter is *diameter* and per-atom density and per-atom mass are defined for particles (e.g. *atom_style granular*), then the mass of each particle is also changed when the diameter changes (density is assumed to stay constant).

For example, these commands would shrink the diameter of all granular particles in the "center" group from 1.0 to 0.1 in a linear fashion over the course of a 1000-step simulation:

```
variable size equal ramp(1.0,0.1)
fix 1 center adapt 10 atom diameter * v_size
```

For *rRESPA time integration*, this fix changes parameters on the outermost rRESPA level.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.2.4 Restrictions

none

16.2.5 Related commands

compute fep, *fix adapt*, *compute ti*, *pair_style */soft*

16.2.6 Default

The option defaults are scale = no, reset = no, after = no.

16.3 fix addforce command

16.3.1 Syntax

```
fix ID group-ID addforce fx fy fz keyword value ...
```

- ID, group-ID are documented in *fix* command
- addforce = style name of this fix command
- fx,fy,fz = force component values (force units)

  ```
  any of fx,fy,fz can be a variable (see below)
  ```

- zero or more keyword/value pairs may be appended to args
- keyword = *every* or *region* or *energy*

```
every value = Nevery
  Nevery = add force every this many timesteps
region value = region-ID
  region-ID = ID of region atoms must be in to have added force
energy value = v_name
  v_name = variable with name that calculates the potential energy of␣
↪each atom in the added force field
```

16.3.2 Examples

```
fix kick flow addforce 1.0 0.0 0.0
fix kick flow addforce 1.0 0.0 v_oscillate
fix ff boundary addforce 0.0 0.0 v_push energy v_espace
```

16.3.3 Description

Add fx,fy,fz to the corresponding component of force for each atom in the group. This command can be used to give an additional push to atoms in a simulation, such as for a simulation of Poiseuille flow in a channel.

Any of the 3 quantities defining the force components can be specified as an equal-style or atom-style *variable*, namely *fx*, *fy*, *fz*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value(s) used to determine the force component.

Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent force field.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent force field with optional time-dependence as well.

If the *every* keyword is used, the *Nevery* setting determines how often the forces are applied. The default value is 1, for every timestep.

If the *region* keyword is used, the atom must also be in the specified geometric *region* in order to have force added to it.

Adding a force to atoms implies a change in their potential energy as they move due to the applied force field. For dynamics via the "run" command, this energy can be optionally added to the system's potential energy for thermodynamic output (see below). For energy minimization via the "minimize" command, this energy must be added to the system's potential energy to formulate a self-consistent minimization problem (see below).

The *energy* keyword is not allowed if the added force is a constant vector F = (fx,fy,fz), with all components defined as numeric constants and not as variables. This is because LAMMPS can compute the energy for each atom directly as E = -x dot F = -(x*fx + y*fy + z*fz), so that -Grad(E) = F.

The *energy* keyword is optional if the added force is defined with one or more variables, and if you are performing dynamics via the *run* command. If the keyword is not used, LAMMPS will set the energy to 0.0, which is typically fine for dynamics.

The *energy* keyword is required if the added force is defined with one or more variables, and you are performing energy minimization via the "minimize" command. The keyword specifies the name of an atom-style *variable* which is used to compute the energy of each atom as function of its position. Like variables used for *fx*, *fy*, *fz*, the energy variable is specified as v_name, where name is the variable name.

Note that when the *energy* keyword is used during an energy minimization, you must insure that the formula defined for the atom-style *variable* is consistent with the force variable formulas, i.e. that -Grad(E) = F. For example, if the force were a spring-like F = kx, then the energy formula should be E = -0.5kx^2. If you don't do this correctly, the minimization will not converge properly.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify energy* option is supported by this fix to add the potential "energy" inferred by the added force to the system's potential energy as part of *thermodynamic output*. This is a fictitious quantity but is needed so that the *minimize* command can include the forces added by this fix in a consistent manner. I.e. there is a decrease in potential energy when atoms move in the direction of the added force.

The *fix_modify virial* option is supported by this fix to add the contribution due to the added forces on atoms to the system's virial as part of *thermodynamic output*. The default is *virial no*

The *fix_modify respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix is adding its forces. Default is the outermost level.

This fix computes a global scalar and a global 3-vector of forces, which can be accessed by various *output commands*. The scalar is the potential energy discussed above. The vector is the total force on the group of atoms before the forces on individual atoms are changed by the fix. The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command. You should not specify force components with a variable that has time-dependence for use with a minimizer, since the minimizer increments the timestep as the iteration count during the minimization.

Note: If you want the fictitious potential energy associated with the added forces to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the *fix_modify energy* option for this fix.

16.3.4 Restrictions

none

16.3.5 Related commands

fix setforce, *fix aveforce*

16.3.6 Default

The option default for the every keyword is every = 1.

16.4 fix addtorque command

16.4.1 Syntax

```
fix ID group-ID addtorque Tx Ty Tz
```

- ID, group-ID are documented in *fix* command
- addtorque = style name of this fix command
- Tx,Ty,Tz = torque component values (torque units)
- any of Tx,Ty,Tz can be a variable (see below)

16.4.2 Examples

```
fix kick bead addtorque 2.0 3.0 5.0
fix kick bead addtorque 0.0 0.0 v_oscillate
```

16.4.3 Description

Add a set of forces to each atom in the group such that:

- the components of the total torque applied on the group (around its center of mass) are Tx,Ty,Tz
- the group would move as a rigid body in the absence of other forces.

This command can be used to drive a group of atoms into rotation.

Any of the 3 quantities defining the torque components can be specified as an equal-style *variable*, namely *Tx*, *Ty*, *Tz*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the torque component.

Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent torque.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify* *energy* option is supported by this fix to add the potential "energy" inferred by the added forces to the system's potential energy as part of *thermodynamic output*. This is a fictitious quantity but is needed so that the *minimize* command can include the forces added by this fix in a consistent manner. I.e. there is a decrease in potential energy when atoms move in the direction of the added forces.

The *fix_modify* *respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix is adding its torque. Default is the outermost level.

This fix computes a global scalar and a global 3-vector, which can be accessed by various *output commands*. The scalar is the potential energy discussed above. The vector is the total torque on the group of atoms before the forces on individual atoms are changed by the fix. The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command. You should not specify force components with a variable that has time-dependence for use with a minimizer, since the minimizer increments the timestep as the iteration count during the minimization.

16.4.4 Restrictions

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.4.5 Related commands

fix addforce

Default: none

16.5 fix append/atoms command

16.5.1 Syntax

```
fix ID group-ID append/atoms face ... keyword value ...
```

- ID, group-ID are documented in *fix* command
- append/atoms = style name of this fix command
- face = *zhi*
- zero or more keyword/value pairs may be appended
- keyword = *basis* or *size* or *freq* or *temp* or *random* or *units*

```
basis values = M itype
  M = which basis atom
  itype = atom type (1-N) to assign to this basis atom
size args = Lz
  Lz = z size of lattice region appended in a single event(distance units)
freq args = freq
  freq = the number of timesteps between append events
temp args = target damp seed extent
```

```
    target = target temperature for the region between zhi-extent and zhi␣
  ↪(temperature units)
    damp = damping parameter (time units)
    seed = random number seed for langevin kicks
    extent = extent of thermostatted region (distance units)
  random args = xmax ymax zmax seed
    xmax, ymax, zmax = maximum displacement in particular direction␣
  ↪(distance units)
    seed = random number seed for random displacement
  units value = lattice or box
    lattice = the wall position is defined in lattice units
    box = the wall position is defined in simulation box units
```

16.5.2 Examples

```
fix 1 all append/atoms zhi size 5.0 freq 295 units lattice
fix 4 all append/atoms zhi size 15.0 freq 5 units box
fix A all append/atoms zhi size 1.0 freq 1000 units lattice
```

16.5.3 Description

This fix creates atoms on a lattice, appended on the zhi edge of the system box. This can be useful when a shock or wave is propagating from zlo. This allows the system to grow with time to accommodate an expanding wave. A simulation box must already exist, which is typically created via the *create_box* command. Before using this command, a lattice must also be defined using the *lattice* command.

This fix will automatically freeze atoms on the zhi edge of the system, so that overlaps are avoided when new atoms are appended.

The *basis* keyword specifies an atom type that will be assigned to specific basis atoms as they are created. See the *lattice* command for specifics on how basis atoms are defined for the unit cell of the lattice. By default, all created atoms are assigned type = 1 unless this keyword specifies differently.

The *size* keyword defines the size in z of the chunk of material to be added.

The *random* keyword will give the atoms random displacements around their lattice points to simulate some initial temperature.

The *temp* keyword will cause a region to be thermostatted with a Langevin thermostat on the zhi boundary. The size of the region is measured from zhi and is set with the *extent* argument.

The *units* keyword determines the meaning of the distance units used to define a wall position, but only when a numeric constant is used. A *box* value selects standard distance units as defined by the *units* command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacings.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.5.4 Restrictions

This fix style is part of the SHOCK package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

The boundary on which atoms are added with append/atoms must be shrink/minimum. The opposite boundary may be any boundary type other than periodic.

16.5.5 Related commands

fix wall/piston command

16.5.6 Default

The keyword defaults are size = 0.0, freq = 0, units = lattice. All added atoms are of type 1 unless the basis keyword is used.

16.6 fix atc command

16.6.1 Syntax

```
fix <fixID> <group> atc <type> <parameter_file>
```

- fixID = name of fix
- group = name of group fix is to be applied
- type = *thermal* or *two_temperature* or *hardy* or *field*

```
thermal = thermal coupling with fields: temperature
two_temperature = electron-phonon coupling with field: temperature and␣
↪electron_temperature
hardy = on-the-fly post-processing using kernel localization functions (see␣
↪"related" section for possible fields)
field = on-the-fly post-processing using mesh-based localization functions␣
↪(see "related" section for possible fields)
```

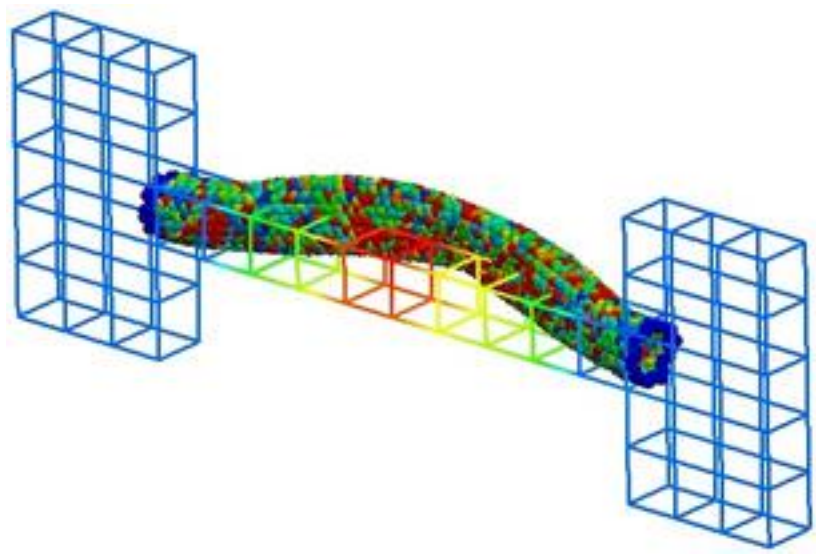
- parameter_file = name of the file with material parameters. Note: Neither hardy nor field requires a parameter file

16.6.2 Examples

```
fix AtC internal atc thermal Ar_thermal.dat
fix AtC internal atc two_temperature Ar_ttm.mat
fix AtC internal atc hardy
fix AtC internal atc field
```

16.6.3 Description

This fix is the beginning to creating a coupled FE/MD simulation and/or an on-the-fly estimation of continuum fields. The coupled versions of this fix do Verlet integration and the post-processing does not. After instantiating this fix, several other fix_modify commands will be needed to set up the problem, e.g. define the finite element mesh and prescribe initial and boundary conditions.



```
The following coupling example is typical, but non-exhaustive:
 # ... commands to create and initialize the MD system

 # initial fix to designate coupling type and group to apply it to
 # tag group physics material_file
 fix AtC internal atc thermal Ar_thermal.mat

 # create a uniform 12 x 2 x 2 mesh that covers region contain the group
 # nx ny nz region periodicity
 fix_modify AtC mesh create 12 2 2 mdRegion f p p

 # specify the control method for the type of coupling
 # physics control_type
 fix_modify AtC thermal control flux

 # specify the initial values for the empirical field "temperature"
 # field node_group value
 fix_modify AtC initial temperature all 30

 # create an output stream for nodal fields
 # filename output_frequency
 fix_modify AtC output atc_fe_output 100

 run 1000
```

likewise for this post-processing example:

```
# ... commands to create and initialize the MD system

# initial fix to designate post-processing and the group to apply it to
# no material file is allowed nor required
```

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(continued from previous page)

```
fix AtC internal atc hardy

# for hardy fix, specific kernel function (function type and range) to # be used as a␣
↪localization function
fix AtC kernel quartic_sphere 10.0

# create a uniform 1 x 1 x 1 mesh that covers region contain the group
# with periodicity this effectively creats a system average
fix_modify AtC mesh create 1 1 1 box p p p

# change from default lagrangian map to eulerian
# refreshed every 100 steps
fix_modify AtC atom_element_map eulerian 100

# start with no field defined
# add mass density, potential energy density, stress and temperature
fix_modify AtC fields add density energy stress temperature

# create an output stream for nodal fields
# filename output_frequency
fix_modify AtC output nvtFE 100 text

run 1000
```

the mesh's linear interpolation functions can be used as the localization function by using the field option:

```
fix AtC internal atc field
fix_modify AtC mesh create 1 1 1 box p p p
...
```

Note coupling and post-processing can be combined in the same simulations using separate fixes.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. The *fix_modify* options relevant to this fix are listed below. No global scalar or vector or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.6.4 Restrictions

Thermal and two_temperature (coupling) types use a Verlet time-integration algorithm. The hardy type does not contain its own time-integrator and must be used with a separate fix that does contain one, e.g. nve, nvt, etc. In addition, currently:

- the coupling is restricted to thermal physics
- the FE computations are done in serial on each processor.

16.6.5 Related commands

After specifying this fix in your input script, several other *fix_modify* commands are used to setup the problem, e.g. define the finite element mesh and prescribe initial and boundary conditions.

fix_modify commands for setup:

- fix_modify AtC mesh create
- fix_modify AtC mesh quadrature
- fix_modify AtC mesh read
- fix_modify AtC mesh write
- fix_modify AtC mesh create_nodeset
- fix_modify AtC mesh add_to_nodeset
- fix_modify AtC mesh create_faceset box
- fix_modify AtC mesh create_faceset plane
- fix_modify AtC mesh create_elementset
- fix_modify AtC mesh delete_elements
- fix_modify AtC mesh nodeset_to_elementset
- fix_modify AtC boundary
- fix_modify AtC internal_quadrature
- fix_modify AtC time_integration (thermal)
- fix_modify AtC time_integration (momentum)
- fix_modify AtC extrinsic electron_integration
- fix_modify AtC internal_element_set
- fix_modify AtC decomposition

fix_modify commands for boundary and initial conditions:

- fix_modify AtC initial
- fix_modify AtC fix
- fix_modify AtC unfix
- fix_modify AtC fix_flux
- fix_modify AtC unfix_flux
- fix_modify AtC source
- fix_modify AtC remove_source

fix_modify commands for control and filtering:

- fix_modify AtC control
- fix_modify AtC control thermal
- fix_modify AtC control thermal correction_max_iterations
- fix_modify AtC control momentum
- fix_modify AtC control localized_lambda

- fix_modify AtC control lumped_lambda_solve
- fix_modify AtC control mask_direction control
- fix_modify AtC filter
- fix_modify AtC filter scale
- fix_modify AtC filter type
- fix_modify AtC equilibrium_start
- fix_modify AtC extrinsic exchange
- fix_modify AtC poisson_solver

fix_modify commands for output:

- fix_modify AtC output
- fix_modify AtC output nodeset
- fix_modify AtC output elementset
- fix_modify AtC output boundary_integral
- fix_modify AtC output contour_integral
- fix_modify AtC mesh output
- fix_modify AtC write_restart
- fix_modify AtC read_restart

fix_modify commands for post-processing:

- fix_modify AtC kernel
- fix_modify AtC fields
- fix_modify AtC grdients
- fix_modify AtC rates
- fix_modify AtC computes
- fix_modify AtC on_the_fly
- fix_modify AtC pair_interactions/bond_interactions
- fix_modify AtC sample_frequency
- fix_modify AtC set

miscellaneous *fix_modify* commands:

- fix_modify AtC atom_element_map
- fix_modify AtC atom_weight
- fix_modify AtC write_atom_weights
- fix_modify AtC reset_time
- fix_modify AtC reset_atomic_reference_positions
- fix_modify AtC fe_md_boundary
- fix_modify AtC boundary_faceset
- fix_modify AtC consistent_fe_initialization

- fix_modify AtC mass_matrix
- fix_modify AtC material
- fix_modify AtC atomic_charge
- fix_modify AtC source_integration
- fix_modify AtC temperature_definition
- fix_modify AtC track_displacement
- fix_modify AtC boundary_dynamics
- fix_modify AtC add_species
- fix_modify AtC add_molecule
- fix_modify AtC remove_species
- fix_modify AtC remove_molecule

Note: a set of example input files with the attendant material files are included with this package

16.6.6 Default

None

For detailed exposition of the theory and algorithms please see:

(Wagner) Wagner, GJ; Jones, RE; Templeton, JA; Parks, MA, "An atomistic-to-continuum coupling method for heat transfer in solids." Special Issue of Computer Methods and Applied Mechanics (2008) 197:3351.

(Zimmerman2004) Zimmerman, JA; Webb, EB; Hoyt, JJ;. Jones, RE; Klein, PA; Bammann, DJ, "Calculation of stress in atomistic simulation." Special Issue of Modelling and Simulation in Materials Science and Engineering (2004), 12:S319.

(Zimmerman2010) Zimmerman, JA; Jones, RE; Templeton, JA, "A material frame approach for evaluating continuum variables in atomistic simulations." Journal of Computational Physics (2010), 229:2364.

(Templeton2010) Templeton, JA; Jones, RE; Wagner, GJ, "Application of a field-based method to spatially varying thermal transport problems in molecular dynamics." Modelling and Simulation in Materials Science and Engineering (2010), 18:085007.

(Jones) Jones, RE; Templeton, JA; Wagner, GJ; Olmsted, D; Modine, JA, "Electron transport enhanced molecular dynamics for metals and semi-metals." International Journal for Numerical Methods in Engineering (2010), 83:940.

(Templeton2011) Templeton, JA; Jones, RE; Lee, JW; Zimmerman, JA; Wong, BM, "A long-range electric field solver for molecular dynamics based on atomistic-to-continuum modeling." Journal of Chemical Theory and Computation (2011), 7:1736.

(Mandadapu) Mandadapu, KK; Templeton, JA; Lee, JW, "Polarization as a field variable from molecular dynamics simulations." Journal of Chemical Physics (2013), 139:054115.

Please refer to the standard finite element (FE) texts, e.g. T.J.R Hughes " The finite element method ", Dover 2003, for the basics of FE simulation.

16.7 fix atom/swap command

16.7.1 Syntax

```
fix ID group-ID atom/swap N X seed T keyword values ...
```

- ID, group-ID are documented in *fix* command
- atom/swap = style name of this fix command
- N = invoke this fix every N steps
- X = number of swaps to attempt every N steps
- seed = random # seed (positive integer)
- T = scaling temperature of the MC swaps (temperature units)
- one or more keyword/value pairs may be appended to args
- keyword = *types* or *mu* or *ke* or *semi-grand* or *region*

```
types values = two or more atom types
mu values = chemical potential of swap types (energy units)
ke value = no or yes
  no = no conservation of kinetic energy after atom swaps
  yes = kinetic energy is conserved after atom swaps
semi-grand value = no or yes
  no = particle type counts and fractions conserved
  yes = semi-grand canonical ensemble, particle fractions not conserved
region value = region-ID
  region-ID = ID of region to use as an exchange/move volume
```

16.7.2 Examples

```
fix 2 all atom/swap 1 1 29494 300.0 ke no types 1 2
fix myFix all atom/swap 100 1 12345 298.0 region my_swap_region types 5 6
fix SGMC all atom/swap 1 100 345 1.0 semi-grand yes types 1 2 3 mu 0.0 4.3 -5.0
```

16.7.3 Description

This fix performs Monte Carlo swaps of atoms of one given atom type with atoms of the other given atom types. The specified T is used in the Metropolis criterion dictating swap probabilities.

Perform X swaps of atoms of one type with atoms of another type according to a Monte Carlo probability. Swap candidates must be in the fix group, must be in the region (if specified), and must be of one of the listed types. Swaps are attempted between candidates that are chosen randomly with equal probability among the candidate atoms. Swaps are not attempted between atoms of the same type since nothing would happen.

All atoms in the simulation domain can be moved using regular time integration displacements, e.g. via *fix nvt*, resulting in a hybrid MC+MD simulation. A smaller-than-usual timestep size may be needed when running such a hybrid simulation, especially if the swapped atoms are not well equilibrated.

The *types* keyword is required. At least two atom types must be specified.

The *ke* keyword can be set to *no* to turn off kinetic energy conservation for swaps. The default is *yes*, which means that swapped atoms have their velocities scaled by the ratio of the masses of the swapped atom types. This ensures

that the kinetic energy of each atom is the same after the swap as it was before the swap, even though the atom masses have changed.

The *semi-grand* keyword can be set to *yes* to switch to the semi-grand canonical ensemble as discussed in *(Sadigh)*. This means that the total number of each particle type does not need to be conserved. The default is *no*, which means that the only kind of swap allowed exchanges an atom of one type with an atom of a different given type. In other words, the relative mole fractions of the swapped atoms remains constant. Whereas in the semi-grand canonical ensemble, the composition of the system can change. Note that when using *semi-grand*, atoms in the fix group whose type is not listed in the *types* keyword are ineligible for attempted conversion. An attempt is made to switch the selected atom (if eligible) to one of the other listed types with equal probability. Acceptance of each attempt depends upon the Metropolis criterion.

The *mu* keyword allows users to specify chemical potentials. This is required and allowed only when using *semi-grand*. All chemical potentials are absolute, so there is one for each swap type listed following the *types* keyword. In semi-grand canonical ensemble simulations the chemical composition of the system is controlled by the difference in these values. So shifting all values by a constant amount will have no effect on the simulation.

This command may optionally use the *region* keyword to define swap volume. The specified region must have been previously defined with a *region* command. It must be defined with side = *in*. Swap attempts occur only between atoms that are both within the specified region. Swaps are not otherwise attempted.

You should ensure you do not swap atoms belonging to a molecule, or LAMMPS will soon generate an error when it tries to find those atoms. LAMMPS will warn you if any of the atoms eligible for swapping have a non-zero molecule ID, but does not check for this at the time of swapping.

If not using *semi-grand* this fix checks to ensure all atoms of the given types have the same atomic charge. LAMMPS doesn't enforce this in general, but it is needed for this fix to simplify the swapping procedure. Successful swaps will swap the atom type and charge of the swapped atoms. Conversely, when using *semi-grand*, it is assumed that all the atom types involved in switches have the same charge. Otherwise, charge would not be conserved. As a consequence, no checks on atomic charges are performed, and successful switches update the atom type but not the atom charge. While it is possible to use *semi-grand* with groups of atoms that have different charges, these charges will not be changed when the atom types change.

Since this fix computes total potential energies before and after proposed swaps, so even complicated potential energy calculations are OK, including the following:

- long-range electrostatics (kspace)
- many body pair styles
- hybrid pair styles
- eam pair styles
- triclinic systems
- need to include potential energy contributions from other fixes

Some fixes have an associated potential energy. Examples of such fixes include: *efield*, *gravity*, *addforce*, *langevin*, *restrain*, *temp/berendsen*, *temp/rescale*, and *wall fixes*. For that energy to be included in the total potential energy of the system (the quantity used when performing GCMC moves), you MUST enable the *fix_modify* *energy* option for that fix. The doc pages for individual *fix* commands specify if this should be done.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the fix to *binary restart files*. This includes information about the random number generator seed, the next timestep for MC exchanges, the number of exchange attempts and successes etc. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

Note: For this to work correctly, the timestep must **not** be changed after reading the restart with *reset_timestep*. The fix will try to detect it and stop with an error.

None of the *fix_modify* options are relevant to this fix.

This fix computes a global vector of length 2, which can be accessed by various *output commands*. The vector values are the following global cumulative quantities:

- 1 = swap attempts
- 2 = swap successes

The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.7.4 Restrictions

This fix is part of the MC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.7.5 Related commands

fix nvt, *neighbor*, *fix deposit*, *fix evaporate*, *delete_atoms*, *fix gcmc*

16.7.6 Default

The option defaults are ke = yes, semi-grand = no, mu = 0.0 for all atom types.

(Sadigh) B Sadigh, P Erhart, A Stukowski, A Caro, E Martinez, and L Zepeda-Ruiz, Phys. Rev. B, 85, 184203 (2012).

16.8 fix ave/atom command

16.8.1 Syntax

```
fix ID group-ID ave/atom Nevery Nrepeat Nfreq value1 value2 ...
```

- ID, group-ID are documented in *fix* command
- ave/atom = style name of this fix command
- Nevery = use input values every this many timesteps
- Nrepeat = # of times to use input values for calculating averages
- Nfreq = calculate averages every this many timesteps one or more input values can be listed
- value = x, y, z, vx, vy, vz, fx, fy, fz, c_ID, c_ID[i], f_ID, f_ID[i], v_name

```
x,y,z,vx,vy,vz,fx,fy,fz = atom attribute (position, velocity, force component)
c_ID = per-atom vector calculated by a compute with ID
c_ID[I] = Ith column of per-atom array calculated by a compute with ID, I can␣
↪include wildcard (see below)
f_ID = per-atom vector calculated by a fix with ID
f_ID[I] = Ith column of per-atom array calculated by a fix with ID, I can include␣
↪wildcard (see below)
v_name = per-atom vector calculated by an atom-style variable with name
```

16.8.2 Examples

```
fix 1 all ave/atom 1 100 100 vx vy vz
fix 1 all ave/atom 10 20 1000 c_my_stress[1]
fix 1 all ave/atom 10 20 1000 c_my_stress[*]
```

16.8.3 Description

Use one or more per-atom vectors as inputs every few timesteps, and average them atom by atom over longer timescales. The resulting per-atom averages can be used by other *output commands* such as the *fix ave/chunk* or *dump custom* commands.

The group specified with the command means only atoms within the group have their averages computed. Results are set to 0.0 for atoms not in the group.

Each input value can be an atom attribute (position, velocity, force component) or can be the result of a *compute* or *fix* or the evaluation of an atom-style *variable*. In the latter cases, the compute, fix, or variable must produce a per-atom vector, not a global quantity or local quantity. If you wish to time-average global quantities from a compute, fix, or variable, then see the *fix ave/time* command.

Each per-atom value of each input vector is averaged independently.

Computes that produce per-atom vectors or arrays are those which have the word *atom* in their style name. See the doc pages for individual *fixes* to determine which ones produce per-atom vectors or arrays. *Variables* of style *atom* are the only ones that can be used with this fix since they produce per-atom vectors.

Note that for values from a compute or fix, the bracketed index I can be specified using a wildcard asterisk with the index to effectively specify multiple values. This takes the form "*" or "*n" or "n*" or "m*n". If N = the size of the vector (for *mode* = scalar) or the number of columns in the array (for *mode* = vector), then an asterisk with no numeric values means all indices from 1 to N. A leading asterisk means all indices from 1 to n (inclusive). A trailing asterisk means all indices from n to N (inclusive). A middle asterisk means all indices from m to n (inclusive).

Using a wildcard is the same as if the individual columns of the array had been listed one by one. E.g. these 2 fix ave/atom commands are equivalent, since the *compute stress/atom* command creates a per-atom array with 6 columns:

```
compute my_stress all stress/atom NULL
fix 1 all ave/atom 10 20 1000 c_my_stress[*]
fix 1 all ave/atom 10 20 1000 c_my_stress[1] c_my_stress[2] &
                              c_my_stress[3] c_my_stress[4] &
                              c_my_stress[5] c_my_stress[6]
```

The *Nevery*, *Nrepeat*, and *Nfreq* arguments specify on what timesteps the input values will be used in order to contribute to the average. The final averaged quantities are generated on timesteps that are a multiple of *Nfreq*. The average is over *Nrepeat* quantities, computed in the preceding portion of the simulation every *Nevery* timesteps. *Nfreq*

must be a multiple of *Nevery* and *Nevery* must be non-zero even if *Nrepeat* is 1. Also, the timesteps contributing to the average value cannot overlap, i.e. Nrepeat*Nevery can not exceed Nfreq.

For example, if Nevery=2, Nrepeat=6, and Nfreq=100, then values on timesteps 90,92,94,96,98,100 will be used to compute the final average on timestep 100. Similarly for timesteps 190,192,194,196,198,200 on timestep 200, etc.

The atom attribute values (x,y,z,vx,vy,vz,fx,fy,fz) are self-explanatory. Note that other atom attributes can be used as inputs to this fix by using the *compute property/atom* command and then specifying an input value from that compute.

Note: The x,y,z attributes are values that are re-wrapped inside the periodic box whenever an atom crosses a periodic boundary. Thus if you time average an atom that spends half its time on either side of the periodic box, you will get a value in the middle of the box. If this is not what you want, consider averaging unwrapped coordinates, which can be provided by the *compute property/atom* command via its xu,yu,zu attributes.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If no bracketed term is appended, the per-atom vector calculated by the compute is used. If a bracketed term containing an index I is appended, the Ith column of the per-atom array calculated by the compute is used. Users can also write code for their own compute styles and *add them to LAMMPS*. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If no bracketed term is appended, the per-atom vector calculated by the fix is used. If a bracketed term containing an index I is appended, the Ith column of the per-atom array calculated by the fix is used. Note that some fixes only produce their values on certain timesteps, which must be compatible with *Nevery*, else an error will result. Users can also write code for their own fix styles and *add them to LAMMPS*. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script as an *atom-style variable* Variables of style *atom* can reference thermodynamic keywords, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of generating per-atom quantities to time average.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global scalar or vector quantities are stored by this fix for access by various *output commands*.

This fix produces a per-atom vector or array which can be accessed by various *output commands*. A vector is produced if only a single quantity is averaged by this fix. If two or more quantities are averaged, then an array of values is produced. The per-atom values can only be accessed on timesteps that are multiples of *Nfreq* since that is when averaging is performed.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.8.4 Restrictions

none

16.8.5 Related commands

compute, *fix ave/histo*, *fix ave/chunk*, *fix ave/time*, *variable*,

Default: none

16.9 fix ave/chunk command

16.9.1 Syntax

```
fix ID group-ID ave/chunk Nevery Nrepeat Nfreq chunkID value1 value2 ... keyword args␣
↪...
```

- ID, group-ID are documented in *fix* command
- ave/chunk = style name of this fix command
- Nevery = use input values every this many timesteps
- Nrepeat = # of times to use input values for calculating averages
- Nfreq = calculate averages every this many timesteps
- chunkID = ID of *compute chunk/atom* command
- one or more input values can be listed
- value = vx, vy, vz, fx, fy, fz, density/mass, density/number, temp, c_ID, c_ID[I], f_ID, f_ID[I], v_name

```
vx,vy,vz,fx,fy,fz = atom attribute (velocity, force component)
density/number, density/mass = number or mass density
temp = temperature
c_ID = per-atom vector calculated by a compute with ID
c_ID[I] = Ith column of per-atom array calculated by a compute with ID, I can␣
↪include wildcard (see below)
f_ID = per-atom vector calculated by a fix with ID
f_ID[I] = Ith column of per-atom array calculated by a fix with ID, I can include␣
↪wildcard (see below)
v_name = per-atom vector calculated by an atom-style variable with name
```

- zero or more keyword/arg pairs may be appended
- keyword = *norm* or *ave* or *bias* or *adof* or *cdof* or *file* or *overwrite* or *title1* or *title2* or *title3*

```
norm arg = all or sample or none = how output on Nfreq steps is␣
↪normalized
  all = output is sum of atoms across all Nrepeat samples, divided by␣
↪atom count
  sample = output is sum of Nrepeat sample averages, divided by Nrepeat
  none = output is sum of Nrepeat sample sums, divided by Nrepeat
ave args = one or running or window M
  one = output new average value every Nfreq steps
  running = output cumulative average of all previous Nfreq steps
  window M = output average of M most recent Nfreq steps
bias arg = bias-ID
  bias-ID = ID of a temperature compute that removes a velocity bias for␣
↪temperature calculation
adof value = dof_per_atom
```

```
    dof_per_atom = define this many degrees-of-freedom per atom for␣
  ↪temperature calculation
  cdof value = dof_per_chunk
    dof_per_chunk = define this many degrees-of-freedom per chunk for␣
  ↪temperature calculation
  file arg = filename
    filename = file to write results to
  overwrite arg = none = overwrite output file with only latest output
  format arg = string
    string = C-style format string
  title1 arg = string
    string = text to print as 1st line of output file
  title2 arg = string
    string = text to print as 2nd line of output file
  title3 arg = string
    string = text to print as 3rd line of output file
```

16.9.2 Examples

```
fix 1 all ave/chunk 10000 1 10000 binchunk c_myCentro title1 "My output values"
fix 1 flow ave/chunk 100 10 1000 molchunk vx vz norm sample file vel.profile
fix 1 flow ave/chunk 100 5 1000 binchunk density/mass ave running
fix 1 flow ave/chunk 100 5 1000 binchunk density/mass ave running
```

NOTE:

If you are trying to replace a deprecated fix ave/spatial command with the newer, more flexible fix ave/chunk and *compute chunk/atom* commands, you simply need to split the fix ave/spatial arguments across the two new commands. For example, this command:

```
fix 1 flow ave/spatial 100 10 1000 y 0.0 1.0 vx vz norm sample file vel.profile
```

could be replaced by:

```
compute cc1 flow chunk/atom bin/1d y 0.0 1.0
fix 1 flow ave/chunk 100 10 1000 cc1 vx vz norm sample file vel.profile
```

16.9.3 Description

Use one or more per-atom vectors as inputs every few timesteps, sum the values over the atoms in each chunk at each timestep, then average the per-chunk values over longer timescales. The resulting chunk averages can be used by other *output commands* such as *thermo_style custom*, and can also be written to a file.

In LAMMPS, chunks are collections of atoms defined by a *compute chunk/atom* command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the *compute chunk/atom* doc page and the *Howto chunk* doc page for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

Note that only atoms in the specified group contribute to the summing and averaging calculations. The *compute chunk/atom* command defines its own group as well as an optional region. Atoms will have a chunk ID = 0, meaning they belong to no chunk, if they are not in that group or region. Thus you can specify the "all" group for this command if you simply want to use the chunk definitions provided by chunkID.

Each specified per-atom value can be an atom attribute (position, velocity, force component), a mass or number density, or the result of a *compute* or *fix* or the evaluation of an atom-style *variable*. In the latter cases, the compute, fix, or variable must produce a per-atom quantity, not a global quantity. Note that the *compute property/atom* command provides access to any attribute defined and stored by atoms. If you wish to time-average global quantities from a compute, fix, or variable, then see the *fix ave/time* command.

The per-atom values of each input vector are summed and averaged independently of the per-atom values in other input vectors.

Computes that produce per-atom quantities are those which have the word *atom* in their style name. See the doc pages for individual *fixes* to determine which ones produce per-atom quantities. *Variables* of style *atom* are the only ones that can be used with this fix since all other styles of variable produce global quantities.

Note that for values from a compute or fix, the bracketed index I can be specified using a wildcard asterisk with the index to effectively specify multiple values. This takes the form "*" or "*n" or "n*" or "m*n". If N = the size of the vector (for *mode* = scalar) or the number of columns in the array (for *mode* = vector), then an asterisk with no numeric values means all indices from 1 to N. A leading asterisk means all indices from 1 to n (inclusive). A trailing asterisk means all indices from n to N (inclusive). A middle asterisk means all indices from m to n (inclusive).

Using a wildcard is the same as if the individual columns of the array had been listed one by one. E.g. these 2 fix ave/chunk commands are equivalent, since the *compute property/atom* command creates, in this case, a per-atom array with 3 columns:

```
compute myAng all property/atom angmomx angmomy angmomz
fix 1 all ave/chunk 100 1 100 cc1 c_myAng[*] file tmp.angmom
fix 2 all ave/chunk 100 1 100 cc1 c_myAng[1] c_myAng[2] c_myAng[3] file tmp.
↪angmom
```

Note: This fix works by creating an array of size *Nchunk* by Nvalues on each processor. *Nchunk* is the number of chunks which is defined by the *compute chunk/atom* command. Nvalues is the number of input values specified. Each processor loops over its atoms, tallying its values to the appropriate chunk. Then the entire array is summed across all processors. This means that using a large number of chunks will incur an overhead in memory and computational cost (summing across processors), so be careful to define a reasonable number of chunks.

The *Nevery*, *Nrepeat*, and *Nfreq* arguments specify on what timesteps the input values will be accessed and contribute to the average. The final averaged quantities are generated on timesteps that are a multiples of *Nfreq*. The average is over *Nrepeat* quantities, computed in the preceding portion of the simulation every *Nevery* timesteps. *Nfreq* must be a multiple of *Nevery* and *Nevery* must be non-zero even if *Nrepeat* is 1. Also, the timesteps contributing to the average value cannot overlap, i.e. Nrepeat*Nevery can not exceed Nfreq.

For example, if Nevery=2, Nrepeat=6, and Nfreq=100, then values on timesteps 90,92,94,96,98,100 will be used to compute the final average on timestep 100. Similarly for timesteps 190,192,194,196,198,200 on timestep 200, etc. If Nrepeat=1 and Nfreq = 100, then no time averaging is done; values are simply generated on timesteps 100,200,etc.

Each input value can also be averaged over the atoms in each chunk. The way the averaging is done across the *Nrepeat* timesteps to produce output on the *Nfreq* timesteps, and across multiple *Nfreq* outputs, is determined by the *norm* and *ave* keyword settings, as discussed below.

Note: To perform per-chunk averaging within a *Nfreq* time window, the number of chunks *Nchunk* defined by the *compute chunk/atom* command must remain constant. If the *ave* keyword is set to *running* or *window* then *Nchunk* must remain constant for the duration of the simulation. This fix forces the chunk/atom compute specified by chunkID to hold *Nchunk* constant for the appropriate time windows, by not allowing it to re-calculate *Nchunk*, which can also affect how it assigns chunk IDs to atoms. This is particularly important to understand if the chunks defined by the *compute chunk/atom* command are spatial bins. If its *units* keyword is set to *box* or *lattice*, then the number of bins *Nchunk* and size of each bin will be fixed over the *Nfreq* time window, which can affect which atoms are discarded if

the simulation box size changes. If its *units* keyword is set to *reduced*, then the number of bins *Nchunk* will still be fixed, but the size of each bin can vary at each timestep if the simulation box size changes, e.g. for an NPT simulation.

The atom attribute values (vx,vy,vz,fx,fy,fz) are self-explanatory. As noted above, any other atom attributes can be used as input values to this fix by using the *compute property/atom* command and then specifying an input value from that compute.

The *density/number* value means the number density is computed for each chunk, i.e. number/volume. The *density/mass* value means the mass density is computed for each chunk, i.e. total-mass/volume. The output values are in units of 1/volume or density (mass/volume). See the *units* command doc page for the definition of density for each choice of units, e.g. gram/cm^3. If the chunks defined by the *compute chunk/atom* command are spatial bins, the volume is the bin volume. Otherwise it is the volume of the entire simulation box.

The *temp* value means the temperature is computed for each chunk, by the formula KE = DOF/2 k T, where KE = total kinetic energy of the chunk of atoms (sum of 1/2 m v^2), DOF = the total number of degrees of freedom for all atoms in the chunk, k = Boltzmann constant, and T = temperature.

The DOF is calculated as N*adof + cdof, where N = number of atoms in the chunk, adof = degrees of freedom per atom, and cdof = degrees of freedom per chunk. By default adof = 2 or 3 = dimensionality of system, as set via the *dimension* command, and cdof = 0.0. This gives the usual formula for temperature.

Note that currently this temperature only includes translational degrees of freedom for each atom. No rotational degrees of freedom are included for finite-size particles. Also no degrees of freedom are subtracted for any velocity bias or constraints that are applied, such as *compute temp/partial*, or *fix shake* or *fix rigid*. This is because those degrees of freedom (e.g. a constrained bond) could apply to sets of atoms that are both included and excluded from a specific chunk, and hence the concept is somewhat ill-defined. In some cases, you can use the *adof* and *cdof* keywords to adjust the calculated degrees of freedom appropriately, as explained below.

Also note that a bias can be subtracted from atom velocities before they are used in the above formula for KE, by using the *bias* keyword. This allows, for example, a thermal temperature to be computed after removal of a flow velocity profile.

Note that the per-chunk temperature calculated by this fix and the *compute temp/chunk* command can be different. The compute calculates the temperature for each chunk for a single snapshot. This fix can do that but can also time average those values over many snapshots, or it can compute a temperature as if the atoms in the chunk on different timesteps were collected together as one set of atoms to calculate their temperature. The compute allows the center-of-mass velocity of each chunk to be subtracted before calculating the temperature; this fix does not.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If no bracketed integer is appended, the per-atom vector calculated by the compute is used. If a bracketed integer is appended, the Ith column of the per-atom array calculated by the compute is used. Users can also write code for their own compute styles and *add them to LAMMPS*. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If no bracketed integer is appended, the per-atom vector calculated by the fix is used. If a bracketed integer is appended, the Ith column of the per-atom array calculated by the fix is used. Note that some fixes only produce their values on certain timesteps, which must be compatible with *Nevery*, else an error results. Users can also write code for their own fix styles and *add them to LAMMPS*. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. Variables of style *atom* can reference thermodynamic keywords and various per-atom attributes, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of generating per-atom quantities to average within chunks.

Additional optional keywords also affect the operation of this fix and its outputs.

The *norm* keyword affects how averaging is done for the per-chunk values that are output every *Nfreq* timesteps.

It the *norm* setting is *all*, which is the default, a chunk value is summed over all atoms in all *Nrepeat* samples, as is the count of atoms in the chunk. The averaged output value for the chunk on the *Nfreq* timesteps is Total-sum / Total-count. In other words it is an average over atoms across the entire *Nfreq* timescale. For the *density/number* and *density/mass* values, the volume (bin volume or system volume) used in the final normalization will be the volume at the final *Nfreq* timestep.

If the *norm* setting is *sample*, the chunk value is summed over atoms for each sample, as is the count, and an "average sample value" is computed for each sample, i.e. Sample-sum / Sample-count. The output value for the chunk on the *Nfreq* timesteps is the average of the *Nrepeat* "average sample values", i.e. the sum of *Nrepeat* "average sample values" divided by *Nrepeat*. In other words it is an average of an average. For the *density/number* and *density/mass* values, the volume (bin volume or system volume) used in the per-sample normalization will be the current volume at each sampling step.

If the *norm* setting is *none*, a similar computation as for the *sample* setting is done, except the individual "average sample values" are "summed sample values". A summed sample value is simply the chunk value summed over atoms in the sample, without dividing by the number of atoms in the sample. The output value for the chunk on the *Nfreq* timesteps is the average of the *Nrepeat* "summed sample values", i.e. the sum of *Nrepeat* "summed sample values" divided by *Nrepeat*. For the *density/number* and *density/mass* values, the volume (bin volume or system volume) used in the per-sample sum normalization will be the current volume at each sampling step.

The *ave* keyword determines how the per-chunk values produced every *Nfreq* steps are averaged with values produced on previous steps that were multiples of *Nfreq*, before they are accessed by another output command or written to a file.

If the *ave* setting is *one*, which is the default, then the chunk values produced on timesteps that are multiples of *Nfreq* are independent of each other; they are output as-is without further averaging.

If the *ave* setting is *running*, then the chunk values produced on timesteps that are multiples of *Nfreq* are summed and averaged in a cumulative sense before being output. Each output chunk value is thus the average of the chunk value produced on that timestep with all preceding values for the same chunk. This running average begins when the fix is defined; it can only be restarted by deleting the fix via the *unfix* command, or re-defining the fix by re-specifying it.

If the *ave* setting is *window*, then the chunk values produced on timesteps that are multiples of *Nfreq* are summed and averaged within a moving "window" of time, so that the last M values for the same chunk are used to produce the output. E.g. if M = 3 and Nfreq = 1000, then the output on step 10000 will be the average of the individual chunk values on steps 8000,9000,10000. Outputs on early steps will average over less than M values if they are not available.

The *bias* keyword specifies the ID of a temperature compute that removes a "bias" velocity from each atom, specified as *bias-ID*. It is only used when the *temp* value is calculated, to compute the thermal temperature of each chunk after the translational kinetic energy components have been altered in a prescribed way, e.g. to remove a flow velocity profile. See the doc pages for individual computes that calculate a temperature to see which ones implement a bias.

The *adof* and *cdof* keywords define the values used in the degree of freedom (DOF) formula described above for temperature calculation for each chunk. They are only used when the *temp* value is calculated. They can be used to calculate a more appropriate temperature for some kinds of chunks. Here are 3 examples:

If spatially binned chunks contain some number of water molecules and *fix shake* is used to make each molecule rigid, then you could calculate a temperature with 6 degrees of freedom (DOF) (3 translational, 3 rotational) per molecule by setting *adof* to 2.0.

If *compute temp/partial* is used with the *bias* keyword to only allow the x component of velocity to contribute to the temperature, then *adof* = 1.0 would be appropriate.

If each chunk consists of a large molecule, with some number of its bonds constrained by *fix shake* or the entire molecule by *fix rigid/small*, *adof* = 0.0 and *cdof* could be set to the remaining degrees of freedom for the entire molecule (entire chunk in this case), e.g. 6 for 3d, or 3 for 2d, for a rigid molecule.

The *file* keyword allows a filename to be specified. Every *Nfreq* timesteps, a section of chunk info will be written to a text file in the following format. A line with the timestep and number of chunks is written. Then one line per chunk is written, containing the chunk ID (1-Nchunk), an optional original ID value, optional coordinate values for chunks that represent spatial bins, the number of atoms in the chunk, and one or more calculated values. More explanation of the optional values is given below. The number of values in each line corresponds to the number of values specified in the fix ave/chunk command. The number of atoms and the value(s) are summed or average quantities, as explained above.

The *overwrite* keyword will continuously overwrite the output file with the latest output, so that it only contains one timestep worth of output. This option can only be used with the *ave running* setting.

The *format* keyword sets the numeric format of each value when it is printed to a file via the *file* keyword. Note that all values are floating point quantities. The default format is %g. You can specify a higher precision if desired, e.g. %20.16g.

The *title1* and *title2* and *title3* keywords allow specification of the strings that will be printed as the first 3 lines of the output file, assuming the *file* keyword was used. LAMMPS uses default values for each of these, so they do not need to be specified.

By default, these header lines are as follows:

```
# Chunk-averaged data for fix ID and group name
# Timestep Number-of-chunks
# Chunk (OrigID) (Coord1) (Coord2) (Coord3) Ncount value1 value2 ...
```

In the first line, ID and name are replaced with the fix-ID and group name. The second line describes the two values that are printed at the first of each section of output. In the third line the values are replaced with the appropriate value names, e.g. fx or c_myCompute[2].

The words in parenthesis only appear with corresponding columns if the chunk style specified for the *compute chunk/atom* command supports them. The OrigID column is only used if the *compress* keyword was set to *yes* for the *compute chunk/atom* command. This means that the original chunk IDs (e.g. molecule IDs) will have been compressed to remove chunk IDs with no atoms assigned to them. Thus a compressed chunk ID of 3 may correspond to an original chunk ID or molecule ID of 415. The OrigID column will list 415 for the 3rd chunk.

The CoordN columns only appear if a *binning* style was used in the *compute chunk/atom* command. For *bin/1d*, *bin/2d*, and *bin/3d* styles the column values are the center point of the bin in the corresponding dimension. Just Coord1 is used for *bin/1d*, Coord2 is added for *bin/2d*, Coord3 is added for *bin/3d*. For *bin/sphere*, just Coord1 is used, and it is the radial coordinate. For *bin/cylinder*, Coord1 and Coord2 are used. Coord1 is the radial coordinate (away from the cylinder axis), and coord2 is the coordinate along the cylinder axis.

Note that if the value of the *units* keyword used in the *compute chunk/atom command* is *box* or *lattice*, the coordinate values will be in distance *units*. If the value of the *units* keyword is *reduced*, the coordinate values will be in unitless reduced units (0-1). This is not true for the Coord1 value of style *bin/sphere* or *bin/cylinder* which both represent radial dimensions. Those values are always in distance *units*.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix computes a global array of values which can be accessed by various *output commands*. The values can only be accessed on timesteps that are multiples of *Nfreq* since that is when averaging is performed. The global array has # of rows = the number of chunks *Nchunk* as calculated by the specified *compute chunk/atom* command. The # of columns = M+1+Nvalues, where M = 1 to 4, depending on whether the optional columns for OrigID and CoordN are used, as explained above. Following the optional columns, the next column contains the count of atoms in the chunk, and the remaining columns are the Nvalue quantities. When the array is accessed with a row I that exceeds the current number of chunks, than a 0.0 is returned by the fix instead of an error, since the number of chunks can vary as a simulation runs depending on how that value is computed by the compute chunk/atom command.

The array values calculated by this fix are treated as "intensive", since they are typically already normalized by the count of atoms in each chunk.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.9.4 Restrictions

none

16.9.5 Related commands

compute, *fix ave/atom*, *fix ave/histo*, *fix ave/time*, *variable*, *fix ave/correlate*

16.9.6 Default

The option defaults are norm = all, ave = one, bias = none, no file output, and title 1,2,3 = strings as described above.

16.10 fix ave/correlate command

16.10.1 Syntax

```
fix ID group-ID ave/correlate Nevery Nrepeat Nfreq value1 value2 ... keyword args ...
```

- ID, group-ID are documented in *fix* command
- ave/correlate = style name of this fix command
- Nevery = use input values every this many timesteps
- Nrepeat = # of correlation time windows to accumulate
- Nfreq = calculate time window averages every this many timesteps
- one or more input values can be listed
- value = c_ID, c_ID[N], f_ID, f_ID[N], v_name

```
c_ID = global scalar calculated by a compute with ID
c_ID[I] = Ith component of global vector calculated by a compute with ID, I can␣
↪include wildcard (see below)
f_ID = global scalar calculated by a fix with ID
f_ID[I] = Ith component of global vector calculated by a fix with ID, I can␣
↪include wildcard (see below)
v_name = global value calculated by an equal-style variable with name
v_name[I] = Ith component of a vector-style variable with name
```

- zero or more keyword/arg pairs may be appended
- keyword = *type* or *ave* or *start* or *prefactor* or *file* or *overwrite* or *title1* or *title2* or *title3*

```
type arg = auto or upper or lower or auto/upper or auto/lower or full
  auto = correlate each value with itself
  upper = correlate each value with each succeeding value
  lower = correlate each value with each preceding value
```

```
    auto/upper = auto + upper
    auto/lower = auto + lower
    full = correlate each value with every other value, including itself =␣
 ↪auto + upper + lower
  ave args = one or running
    one = zero the correlation accumulation every Nfreq steps
    running = accumulate correlations continuously
  start args = Nstart
    Nstart = start accumulating correlations on this timestep
  prefactor args = value
    value = prefactor to scale all the correlation data by
  file arg = filename
    filename = name of file to output correlation data to
  overwrite arg = none = overwrite output file with only latest output
  title1 arg = string
    string = text to print as 1st line of output file
  title2 arg = string
    string = text to print as 2nd line of output file
  title3 arg = string
    string = text to print as 3rd line of output file
```

16.10.2 Examples

```
fix 1 all ave/correlate 5 100 1000 c_myTemp file temp.correlate
fix 1 all ave/correlate 1 50 10000 &
          c_thermo_press[1] c_thermo_press[2] c_thermo_press[3] &
          type upper ave running title1 "My correlation data"
```

fix 1 all ave/correlate 1 50 10000 c_thermo_press[*]

16.10.3 Description

Use one or more global scalar values as inputs every few timesteps, calculate time correlations between them at varying time intervals, and average the correlation data over longer timescales. The resulting correlation values can be time integrated by *variables* or used by other *output commands* such as *thermo_style custom*, and can also be written to a file. See the *fix ave/correlate/long* command for an alternate method for computing correlation functions efficiently over very long time windows.

The group specified with this command is ignored. However, note that specified values may represent calculations performed by computes and fixes which store their own "group" definitions.

Each listed value can be the result of a *compute* or *fix* or the evaluation of an equal-style or vector-style *variable*. In each case, the compute, fix, or variable must produce a global quantity, not a per-atom or local quantity. If you wish to spatial- or time-average or histogram per-atom quantities from a compute, fix, or variable, then see the *fix ave/chunk*, *fix ave/atom*, or *fix ave/histo* commands. If you wish to convert a per-atom quantity into a single global value, see the *compute reduce* command.

The input values must either be all scalars. What kinds of correlations between input values are calculated is determined by the *type* keyword as discussed below.

Computes that produce global quantities are those which do not have the word *atom* in their style name. Only a few *fixes* produce global quantities. See the doc pages for individual fixes for info on which ones produce such values. *Variables* of style *equal* and *vector* are the only ones that can be used with this fix. Variables of style *atom* cannot be used, since they produce per-atom values.

Note that for values from a compute or fix, the bracketed index I can be specified using a wildcard asterisk with the index to effectively specify multiple values. This takes the form "*" or "*n" or "n*" or "m*n". If N = the size of the vector (for *mode* = scalar) or the number of columns in the array (for *mode* = vector), then an asterisk with no numeric values means all indices from 1 to N. A leading asterisk means all indices from 1 to n (inclusive). A trailing asterisk means all indices from n to N (inclusive). A middle asterisk means all indices from m to n (inclusive).

Using a wildcard is the same as if the individual elements of the vector had been listed one by one. E.g. these 2 fix ave/correlate commands are equivalent, since the *compute pressure* command creates a global vector with 6 values.

```
compute myPress all pressure NULL
fix 1 all ave/correlate 1 50 10000 c_myPress[*]
fix 1 all ave/correlate 1 50 10000 &
          c_myPress[1] c_myPress[2] c_myPress[3] &
          c_myPress[4] c_myPress[5] c_myPress[6]
```

The *Nevery*, *Nrepeat*, and *Nfreq* arguments specify on what timesteps the input values will be used to calculate correlation data. The input values are sampled every *Nevery* timesteps. The correlation data for the preceding samples is computed on timesteps that are a multiple of *Nfreq*. Consider a set of samples from some initial time up to an output timestep. The initial time could be the beginning of the simulation or the last output time; see the *ave* keyword for options. For the set of samples, the correlation value Cij is calculated as:

```
Cij(delta) = ave(Vi(t)*Vj(t+delta))
```

which is the correlation value between input values Vi and Vj, separated by time delta. Note that the second value Vj in the pair is always the one sampled at the later time. The ave() represents an average over every pair of samples in the set that are separated by time delta. The maximum delta used is of size (*Nrepeat*-1)**Nevery*. Thus the correlation between a pair of input values yields *Nrepeat* correlation datums:

```
Cij(0), Cij(Nevery), Cij(2*Nevery), ..., Cij((Nrepeat-1)*Nevery)
```

For example, if Nevery=5, Nrepeat=6, and Nfreq=100, then values on timesteps 0,5,10,15,…,100 will be used to compute the final averages on timestep 100. Six averages will be computed: Cij(0), Cij(5), Cij(10), Cij(15), Cij(20), and Cij(25). Cij(10) on timestep 100 will be the average of 19 samples, namely Vi(0)*Vj(10), Vi(5)*Vj(15), Vi(10)*Vj20), Vi(15)*Vj(25), …, Vi(85)*Vj(95), Vi(90)*Vj(100).

Nfreq must be a multiple of *Nevery*; *Nevery* and *Nrepeat* must be non-zero. Also, if the *ave* keyword is set to *one* which is the default, then *Nfreq* >= (*Nrepeat*-1)**Nevery* is required.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If no bracketed term is appended, the global scalar calculated by the compute is used. If a bracketed term is appended, the Ith element of the global vector calculated by the compute is used. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

Note that there is a *compute reduce* command which can sum per-atom quantities into a global scalar or vector which can thus be accessed by fix ave/correlate. Or it can be a compute defined not in your input script, but by *thermodynamic output* or other fixes such as *fix nvt* or *fix temp/rescale*. See the doc pages for these commands which give the IDs of these computes. Users can also write code for their own compute styles and *add them to LAMMPS*.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If no bracketed term is appended, the global scalar calculated by the fix is used. If a bracketed term is appended, the Ith element of the global vector calculated by the fix is used. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

Note that some fixes only produce their values on certain timesteps, which must be compatible with *Nevery*, else an error will result. Users can also write code for their own fix styles and *add them to LAMMPS*.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. Only equal-style or vector-style variables can be referenced; the latter requires a bracketed term to specify the Ith element of

the vector calculated by the variable. See the *variable* command for details. Note that variables of style *equal* or *vector* define a formula which can reference individual atom properties or thermodynamic keywords, or they can invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of specifying quantities to time correlate.

Additional optional keywords also affect the operation of this fix.

The *type* keyword determines which pairs of input values are correlated with each other. For N input values Vi, for i = 1 to N, let the number of pairs = Npair. Note that the second value in the pair Vi(t)*Vj(t+delta) is always the one sampled at the later time.

- If *type* is set to *auto* then each input value is correlated with itself. I.e. Cii = Vi*Vi, for i = 1 to N, so Npair = N.
- If *type* is set to *upper* then each input value is correlated with every succeeding value. I.e. Cij = Vi*Vj, for i < j, so Npair = N*(N-1)/2.
- If *type* is set to *lower* then each input value is correlated with every preceding value. I.e. Cij = Vi*Vj, for i > j, so Npair = N*(N-1)/2.
- If *type* is set to *auto/upper* then each input value is correlated with itself and every succeeding value. I.e. Cij = Vi*Vj, for i >= j, so Npair = N*(N+1)/2.
- If *type* is set to *auto/lower* then each input value is correlated with itself and every preceding value. I.e. Cij = Vi*Vj, for i <= j, so Npair = N*(N+1)/2.
- If *type* is set to *full* then each input value is correlated with itself and every other value. I.e. Cij = Vi*Vj, for i,j = 1,N so Npair = N^2.

The *ave* keyword determines what happens to the accumulation of correlation samples every *Nfreq* timesteps. If the *ave* setting is *one*, then the accumulation is restarted or zeroed every *Nfreq* timesteps. Thus the outputs on successive *Nfreq* timesteps are essentially independent of each other. The exception is that the Cij(0) = Vi(T)*Vj(T) value at a timestep T, where T is a multiple of *Nfreq*, contributes to the correlation output both at time T and at time T+Nfreq.

If the *ave* setting is *running*, then the accumulation is never zeroed. Thus the output of correlation data at any timestep is the average over samples accumulated every *Nevery* steps since the fix was defined. it can only be restarted by deleting the fix via the *unfix* command, or by re-defining the fix by re-specifying it.

The *start* keyword specifies what timestep the accumulation of correlation samples will begin on. The default is step 0. Setting it to a larger value can avoid adding non-equilibrated data to the correlation averages.

The *prefactor* keyword specifies a constant which will be used as a multiplier on the correlation data after it is averaged. It is effectively a scale factor on Vi*Vj, which can be used to account for the size of the time window or other unit conversions.

The *file* keyword allows a filename to be specified. Every *Nfreq* steps, an array of correlation data is written to the file. The number of rows is *Nrepeat*, as described above. The number of columns is the Npair+2, also as described above. Thus the file ends up to be a series of these array sections.

The *overwrite* keyword will continuously overwrite the output file with the latest output, so that it only contains one timestep worth of output. This option can only be used with the *ave running* setting.

The *title1* and *title2* and *title3* keywords allow specification of the strings that will be printed as the first 3 lines of the output file, assuming the *file* keyword was used. LAMMPS uses default values for each of these, so they do not need to be specified.

By default, these header lines are as follows:

```
# Time-correlated data for fix ID
# TimeStep Number-of-time-windows
# Index TimeDelta Ncount valueI*valueJ valueI*valueJ ...
```

In the first line, ID is replaced with the fix-ID. The second line describes the two values that are printed at the first of each section of output. In the third line the value pairs are replaced with the appropriate fields from the fix ave/correlate command.

Let Sij = a set of time correlation data for input values I and J, namely the *Nrepeat* values:

```
Sij = Cij(0), Cij(Nevery), Cij(2*Nevery), ..., Cij(*Nrepeat-1)*Nevery)
```

As explained below, these datums are output as one column of a global array, which is effectively the correlation matrix.

The *trap* function defined for *equal-style variables* can be used to perform a time integration of this vector of datums, using a trapezoidal rule. This is useful for calculating various quantities which can be derived from time correlation data. If a normalization factor is needed for the time integration, it can be included in the variable formula or via the *prefactor* keyword.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix computes a global array of values which can be accessed by various *output commands*. The values can only be accessed on timesteps that are multiples of *Nfreq* since that is when averaging is performed. The global array has # of rows = *Nrepeat* and # of columns = Npair+2. The first column has the time delta (in timesteps) between the pairs of input values used to calculate the correlation, as described above. The 2nd column has the number of samples contributing to the correlation average, as described above. The remaining Npair columns are for I,J pairs of the N input values, as determined by the *type* keyword, as described above.

- For *type* = *auto*, the Npair = N columns are ordered: C11, C22, . . . , CNN.
- For *type* = *upper*, the Npair = N*(N-1)/2 columns are ordered: C12, C13, . . . , C1N, C23, . . . , C2N, C34, . . . , CN-1N.
- For *type* = *lower*, the Npair = N*(N-1)/2 columns are ordered: C21, C31, C32, C41, C42, C43, . . . , CN1, CN2, . . . , CNN-1.
- For *type* = *auto/upper*, the Npair = N*(N+1)/2 columns are ordered: C11, C12, C13, . . . , C1N, C22, C23, . . . , C2N, C33, C34, . . . , CN-1N, CNN.
- For *type* = *auto/lower*, the Npair = N*(N+1)/2 columns are ordered: C11, C21, C22, C31, C32, C33, C41, . . . , C44, CN1, CN2, . . . , CNN-1, CNN.
- For *type* = *full*, the Npair = N^2 columns are ordered: C11, C12, . . . , C1N, C21, C22, . . . , C2N, C31, . . . , C3N, . . . , CN1, . . . , CNN-1, CNN.

The array values calculated by this fix are treated as intensive. If you need to divide them by the number of atoms, you must do this in a later processing step, e.g. when using them in a *variable*.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.10.4 Restrictions

none

16.10.5 Related commands

fix ave/correlate/long, *compute*, *fix ave/time*, *fix ave/atom*, *fix ave/chunk*, *fix ave/histo*, *variable*

Default: none

The option defaults are ave = one, type = auto, start = 0, no file output, title 1,2,3 = strings as described above, and prefactor = 1.0.

16.11 fix ave/correlate/long command

16.11.1 Syntax

```
fix ID group-ID ave/correlate/long Nevery Nfreq value1 value2 ... keyword args ...
```

- ID, group-ID are documented in *fix* command
- ave/correlate/long = style name of this fix command
- Nevery = use input values every this many timesteps
- Nfreq = save state of the time correlation functions every this many timesteps
- one or more input values can be listed
- value = c_ID, c_ID[N], f_ID, f_ID[N], v_name

```
c_ID = global scalar calculated by a compute with ID
c_ID[I] = Ith component of global vector calculated by a compute with ID
f_ID = global scalar calculated by a fix with ID
f_ID[I] = Ith component of global vector calculated by a fix with ID
v_name = global value calculated by an equal-style variable with name
```

- zero or more keyword/arg pairs may be appended
- keyword = *type* or *start* or *file* or *overwrite* or *title1* or *title2* or *ncorr* or *p* or *m*

```
type arg = auto or upper or lower or auto/upper or auto/lower or full
  auto = correlate each value with itself
  upper = correlate each value with each succeeding value
  lower = correlate each value with each preceding value
  auto/upper = auto + upper
  auto/lower = auto + lower
  full = correlate each value with every other value, including itself =␣
↪auto + upper + lower
start args = Nstart
  Nstart = start accumulating correlations on this timestep
file arg = filename
  filename = name of file to output correlation data to
overwrite arg = none = overwrite output file with only latest output
title1 arg = string
  string = text to print as 1st line of output file
```

```
title2 arg = string
  string = text to print as 2nd line of output file
ncorr arg = Ncorrelators
  Ncorrelators = number of correlators to store
nlen args = Nlen
  Nlen = length of each correlator
ncount args = Ncount
  Ncount = number of values over which succesive correlators are averaged
```

16.11.2 Examples

```
fix 1 all ave/correlate/long 5 1000 c_myTemp file temp.correlate
fix 1 all ave/correlate/long 1 10000 &
          c_thermo_press[1] c_thermo_press[2] c_thermo_press[3] &
          type upper title1 "My correlation data" nlen 15 ncount 3
```

16.11.3 Description

This fix is similar in spirit and syntax to the *fix ave/correlate*. However, this fix allows the efficient calculation of time correlation functions on-the-fly over extremely long time windows with little additional CPU overhead, using a multiple-tau method *(Ramirez)* that decreases the resolution of the stored correlation function with time. It is not a full drop-in replacement.

The group specified with this command is ignored. However, note that specified values may represent calculations performed by computes and fixes which store their own "group" definitions.

Each listed value can be the result of a compute or fix or the evaluation of an equal-style variable. See the *fix ave/correlate* doc page for details.

The *Nevery* and *Nfreq* arguments specify on what timesteps the input values will be used to calculate correlation data, and the frequency with which the time correlation functions will be output to a file. Note that there is no *Nrepeat* argument, unlike the *fix ave/correlate* command.

The optional keywords *ncorr*, *nlen*, and *ncount* are unique to this command and determine the number of correlation points calculated and the memory and CPU overhead used by this calculation. *Nlen* and *ncount* determine the amount of averaging done at longer correlation times. The default values *nlen=16*, *ncount=2* ensure that the systematic error of the multiple-tau correlator is always below the level of the statistical error of a typical simulation (which depends on the ensemble size and the simulation length).

The maximum correlation time (in time steps) that can be reached is given by the formula (nlen-1) * ncount^(ncorr-1). Longer correlation times are discarded and not calculated. With the default values of the parameters (ncorr=20, nlen=16 and ncount=2), this corresponds to 7864320 time steps. If longer correlation times are needed, the value of ncorr should be increased. Using nlen=16 and ncount=2, with ncorr=30, the maximum number of steps that can be correlated is 80530636808. If ncorr=40, correlation times in excess of 8e12 time steps can be calculated.

The total memory needed for each correlation pair is roughly 4*ncorr*nlen*8 bytes. With the default values of the parameters, this corresponds to about 10 KB.

For the meaning of the additional optional keywords, see the *fix ave/correlate* doc page.

Restart, fix_modify, output, run start/stop, minimize info:

Contrary to *fix ave/correlate* this fix does **not** provide access to its internal data to various output options. Since this fix in intended for the calculation of time correlation functions over very long MD simulations, the information about this fix is written automatically to binary restart files, so that the time correlation calculation can continue in subsequent simulations. None of the fix_modify options are relevant to this fix.

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

16.11.4 Restrictions

This compute is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.11.5 Related commands

fix ave/correlate

Default: none

The option defaults for keywords that are also keywords for the *fix ave/correlate* command are as follows: type = auto, start = 0, no file output, title 1,2 = strings as described on the *fix ave/correlate* doc page.

The option defaults for keywords unique to this command are as follows: ncorr=20, nlen=16, ncount=2.

(Ramirez) J. Ramirez, S.K. Sukumaran, B. Vorselaars and A.E. Likhtman, J. Chem. Phys. 133, 154103 (2010).

16.12 fix ave/histo command

16.13 fix ave/histo/weight command

16.13.1 Syntax

```
fix ID group-ID style Nevery Nrepeat Nfreq lo hi Nbin value1 value2 ... keyword args .
↪..
```

- ID, group-ID are documented in *fix* command
- style = *ave/histo* or *ave/histo/weight* = style name of this fix command
- Nevery = use input values every this many timesteps
- Nrepeat = # of times to use input values for calculating histogram
- Nfreq = calculate histogram every this many timesteps
- lo,hi = lo/hi bounds within which to histogram
- Nbin = # of histogram bins
- one or more input values can be listed
- value = x, y, z, vx, vy, vz, fx, fy, fz, c_ID, c_ID[N], f_ID, f_ID[N], v_name

```
x,y,z,vx,vy,vz,fx,fy,fz = atom attribute (position, velocity, force component)
c_ID = scalar or vector calculated by a compute with ID
c_ID[I] = Ith component of vector or Ith column of array calculated by a compute␣
↪with ID, I can include wildcard (see below)
f_ID = scalar or vector calculated by a fix with ID
```

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```
f_ID[I] = Ith component of vector or Ith column of array calculated by a fix with␣
↪ID, I can include wildcard (see below)
v_name = value(s) calculated by an equal-style or vector-style or atom-style␣
↪variable with name
v_name[I] = value calculated by a vector-style variable with name
```

- zero or more keyword/arg pairs may be appended
- keyword = *mode* or *file* or *ave* or *start* or *beyond* or *overwrite* or *title1* or *title2* or *title3*

```
mode arg = scalar or vector
  scalar = all input values are scalars
  vector = all input values are vectors
kind arg = global or peratom or local
file arg = filename
  filename = name of file to output histogram(s) to
ave args = one or running or window
  one = output a new average value every Nfreq steps
  running = output cumulative average of all previous Nfreq steps
  window M = output average of M most recent Nfreq steps
start args = Nstart
  Nstart = start averaging on this timestep
beyond arg = ignore or end or extra
  ignore = ignore values outside histogram lo/hi bounds
  end = count values outside histogram lo/hi bounds in end bins
  extra = create 2 extra bins for value outside histogram lo/hi bounds
overwrite arg = none = overwrite output file with only latest output
title1 arg = string
  string = text to print as 1st line of output file
title2 arg = string
  string = text to print as 2nd line of output file
title3 arg = string
  string = text to print as 3rd line of output file, only for vector mode
```

16.13.2 Examples

```
fix 1 all ave/histo 100 5 1000 0.5 1.5 50 c_myTemp file temp.histo ave running
fix 1 all ave/histo 100 5 1000 -5 5 100 c_thermo_press[2] c_thermo_press[3]␣
↪title1 "My output values"
fix 1 all ave/histo 100 5 1000 -5 5 100 c_thermo_press[*]
fix 1 all ave/histo 1 100 1000 -2.0 2.0 18 vx vy vz mode vector ave running␣
↪beyond extra
fix 1 all ave/histo/weight 1 1 1 10 100 2000 c_XRD[1] c_XRD[2]
```

16.13.3 Description

Use one or more values as inputs every few timesteps to create a single histogram. The histogram can then be averaged over longer timescales. The resulting histogram can be used by other *output commands*, and can also be written to a file. The fix ave/histo/weight command has identical syntax to fix ave/histo, except that exactly two values must be specified. See details below.

The group specified with this command is ignored for global and local input values. For per-atom input values, only atoms in the group contribute to the histogram. Note that regardless of the specified group, specified values may represent calculations performed by computes and fixes which store their own "group" definition.

A histogram is simply a count of the number of values that fall within a histogram bin. *Nbins* are defined, with even spacing between *lo* and *hi*. Values that fall outside the lo/hi bounds can be treated in different ways; see the discussion of the *beyond* keyword below.

Each input value can be an atom attribute (position, velocity, force component) or can be the result of a *compute* or *fix* or the evaluation of an equal-style or vector-style or atom-style *variable*. The set of input values can be either all global, all per-atom, or all local quantities. Inputs of different kinds (e.g. global and per-atom) cannot be mixed. Atom attributes are per-atom vector values. See the doc page for individual "compute" and "fix" commands to see what kinds of quantities they generate. See the optional *kind* keyword below for how to force the fix ave/histo command to disambiguate if necessary.

Note that the output of this command is a single histogram for all input values combined together, not one histogram per input value. See below for details on the format of the output of this fix.

The input values must either be all scalars or all vectors (or arrays), depending on the setting of the *mode* keyword.

If *mode* = scalar, then the input values must be scalars, or vectors with a bracketed term appended, indicating the Ith value of the vector is used.

If *mode* = vector, then the input values must be vectors, or arrays with a bracketed term appended, indicating the Ith column of the array is used.

Note that for values from a compute or fix, the bracketed index I can be specified using a wildcard asterisk with the index to effectively specify multiple values. This takes the form "*" or "*n" or "n*" or "m*n". If N = the size of the vector (for *mode* = scalar) or the number of columns in the array (for *mode* = vector), then an asterisk with no numeric values means all indices from 1 to N. A leading asterisk means all indices from 1 to n (inclusive). A trailing asterisk means all indices from n to N (inclusive). A middle asterisk means all indices from m to n (inclusive).

Using a wildcard is the same as if the individual elements of the vector or columns of the array had been listed one by one. E.g. these 2 fix ave/histo commands are equivalent, since the *compute com/chunk* command creates a global array with 3 columns:

```
compute myCOM all com/chunk
fix 1 all ave/histo 100 1 100 c_myCOM[*] file tmp1.com mode vector
fix 2 all ave/histo 100 1 100 c_myCOM[1] c_myCOM[2] c_myCOM[3] file tmp2.com␣
↪mode vector
```

If the fix ave/histo/weight command is used, exactly two values must be specified. If the values are vectors, they must be the same length. The first value (a scalar or vector) is what is histogrammed into bins, in the same manner the fix ave/histo command operates. The second value (a scalar or vector) is used as a "weight". This means that instead of each value tallying a "1" to its bin, the corresponding weight is tallied. E.g. The Nth entry (weight) in the second vector is tallied to the bin corresponding to the Nth entry in the first vector.

The *Nevery*, *Nrepeat*, and *Nfreq* arguments specify on what timesteps the input values will be used in order to contribute to the histogram. The final histogram is generated on timesteps that are multiple of *Nfreq*. It is averaged over *Nrepeat* histograms, computed in the preceding portion of the simulation every *Nevery* timesteps. *Nfreq* must

be a multiple of *Nevery* and *Nevery* must be non-zero even if *Nrepeat* is 1. Also, the timesteps contributing to the histogram value cannot overlap, i.e. Nrepeat*Nevery can not exceed Nfreq.

For example, if Nevery=2, Nrepeat=6, and Nfreq=100, then input values on timesteps 90,92,94,96,98,100 will be used to compute the final histogram on timestep 100. Similarly for timesteps 190,192,194,196,198,200 on timestep 200, etc. If Nrepeat=1 and Nfreq = 100, then no time averaging of the histogram is done; a histogram is simply generated on timesteps 100,200,etc.

The atom attribute values (x,y,z,vx,vy,vz,fx,fy,fz) are self-explanatory. Note that other atom attributes can be used as inputs to this fix by using the *compute property/atom* command and then specifying an input value from that compute.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If *mode* = scalar, then if no bracketed term is appended, the global scalar calculated by the compute is used. If a bracketed term is appended, the Ith element of the global vector calculated by the compute is used. If *mode* = vector, then if no bracketed term is appended, the global or per-atom or local vector calculated by the compute is used. If a bracketed term is appended, the Ith column of the global or per-atom or local array calculated by the compute is used. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

Note that there is a *compute reduce* command which can sum per-atom quantities into a global scalar or vector which can thus be accessed by fix ave/histo. Or it can be a compute defined not in your input script, but by *thermodynamic output* or other fixes such as *fix nvt* or *fix temp/rescale*. See the doc pages for these commands which give the IDs of these computes. Users can also write code for their own compute styles and *add them to LAMMPS*.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If *mode* = scalar, then if no bracketed term is appended, the global scalar calculated by the fix is used. If a bracketed term is appended, the Ith element of the global vector calculated by the fix is used. If *mode* = vector, then if no bracketed term is appended, the global or per-atom or local vector calculated by the fix is used. If a bracketed term is appended, the Ith column of the global or per-atom or local array calculated by the fix is used. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

Note that some fixes only produce their values on certain timesteps, which must be compatible with *Nevery*, else an error will result. Users can also write code for their own fix styles and *add them to LAMMPS*.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. If *mode* = scalar, then only equal-style or vector-style variables can be used, which both produce global values. In this mode, a vector-style variable requires a bracketed term to specify the Ith element of the vector calculated by the variable. If *mode* = vector, then only vector-style or atom-style variables can be used, which produce a global or per-atom vector respectively. The vector-style variable must be used without a bracketed term. See the *variable* command for details.

Note that variables of style *equal*, *vector*, and *atom* define a formula which can reference individual atom properties or thermodynamic keywords, or they can invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of specifying quantities to histogram.

Additional optional keywords also affect the operation of this fix.

If the *mode* keyword is set to *scalar*, then all input values must be global scalars, or elements of global vectors. If the *mode* keyword is set to *vector*, then all input values must be global or per-atom or local vectors, or columns of global or per-atom or local arrays.

The *kind* keyword only needs to be set if a compute or fix produces more than one kind of output (global, per-atom, local). If this is not the case, then LAMMPS will determine what kind of input is provided and whether all the input arguments are consistent. If a compute or fix produces more than one kind of output, the *kind* keyword should be used to specify which output will be used. The remaining input arguments must still be consistent.

The *beyond* keyword determines how input values that fall outside the *lo* to *hi* bounds are treated. Values such that *lo* <= value <= *hi* are assigned to one bin. Values on a bin boundary are assigned to the lower of the 2 bins. If *beyond* is set to *ignore* then values < *lo* and values > *hi* are ignored, i.e. they are not binned. If *beyond* is set to *end* then values <

lo are counted in the first bin and values > *hi* are counted in the last bin. If *beyond* is set to *extend* then two extra bins are created, so that there are Nbins+2 total bins. Values < *lo* are counted in the first bin and values > *hi* are counted in the last bin (Nbins+2). Values between *lo* and *hi* (inclusive) are counted in bins 2 through Nbins+1. The "coordinate" stored and printed for these two extra bins is *lo* and *hi*.

The *ave* keyword determines how the histogram produced every *Nfreq* steps are averaged with histograms produced on previous steps that were multiples of *Nfreq*, before they are accessed by another output command or written to a file.

If the *ave* setting is *one*, then the histograms produced on timesteps that are multiples of *Nfreq* are independent of each other; they are output as-is without further averaging.

If the *ave* setting is *running*, then the histograms produced on timesteps that are multiples of *Nfreq* are summed and averaged in a cumulative sense before being output. Each bin value in the histogram is thus the average of the bin value produced on that timestep with all preceding values for the same bin. This running average begins when the fix is defined; it can only be restarted by deleting the fix via the *unfix* command, or by re-defining the fix by re-specifying it.

If the *ave* setting is *window*, then the histograms produced on timesteps that are multiples of *Nfreq* are summed within a moving "window" of time, so that the last M histograms are used to produce the output. E.g. if M = 3 and Nfreq = 1000, then the output on step 10000 will be the combined histogram of the individual histograms on steps 8000,9000,10000. Outputs on early steps will be sums over less than M histograms if they are not available.

The *start* keyword specifies what timestep histogramming will begin on. The default is step 0. Often input values can be 0.0 at time 0, so setting *start* to a larger value can avoid including a 0.0 in a running or windowed histogram.

The *file* keyword allows a filename to be specified. Every *Nfreq* steps, one histogram is written to the file. This includes a leading line that contains the timestep, number of bins, the total count of values contributing to the histogram, the count of values that were not histogrammed (see the *beyond* keyword), the minimum value encountered, and the maximum value encountered. The min/max values include values that were not histogrammed. Following the leading line, one line per bin is written into the file. Each line contains the bin #, the coordinate for the center of the bin (between *lo* and *hi*), the count of values in the bin, and the normalized count. The normalized count is the bin count divided by the total count (not including values not histogrammed), so that the normalized values sum to 1.0 across all bins.

The *overwrite* keyword will continuously overwrite the output file with the latest output, so that it only contains one timestep worth of output. This option can only be used with the *ave running* setting.

The *title1* and *title2* and *title3* keywords allow specification of the strings that will be printed as the first 3 lines of the output file, assuming the *file* keyword was used. LAMMPS uses default values for each of these, so they do not need to be specified.

By default, these header lines are as follows:

```
# Histogram for fix ID
# TimeStep Number-of-bins Total-counts Missing-counts Min-value Max-value
# Bin Coord Count Count/Total
```

In the first line, ID is replaced with the fix-ID. The second line describes the six values that are printed at the first of each section of output. The third describes the 4 values printed for each bin in the histogram.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix produces a global vector and global array which can be accessed by various *output commands*. The values can only be accessed on timesteps that are multiples of *Nfreq* since that is when a histogram is generated. The global vector has 4 values:

- 1 = total counts in the histogram
- 2 = values that were not histogrammed (see *beyond* keyword)
- 3 = min value of all input values, including ones not histogrammed
- 4 = max value of all input values, including ones not histogrammed

The global array has # of rows = Nbins and # of columns = 3. The first column has the bin coordinate, the 2nd column has the count of values in that histogram bin, and the 3rd column has the bin count divided by the total count (not including missing counts), so that the values in the 3rd column sum to 1.0.

The vector and array values calculated by this fix are all treated as intensive. If this is not the case, e.g. due to histogramming per-atom input values, then you will need to account for that when interpreting the values produced by this fix.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.13.4 Restrictions

none

16.13.5 Related commands

compute, *fix ave/atom*, *fix ave/chunk*, *fix ave/time*, *variable*, *fix ave/correlate*,

Default: none

The option defaults are mode = scalar, kind = figured out from input arguments, ave = one, start = 0, no file output, beyond = ignore, and title 1,2,3 = strings as described above.

16.14 fix ave/time command

16.14.1 Syntax

```
fix ID group-ID ave/time Nevery Nrepeat Nfreq value1 value2 ... keyword args ...
```

- ID, group-ID are documented in *fix* command
- ave/time = style name of this fix command
- Nevery = use input values every this many timesteps
- Nrepeat = # of times to use input values for calculating averages
- Nfreq = calculate averages every this many timesteps
- one or more input values can be listed
- value = c_ID, c_ID[N], f_ID, f_ID[N], v_name

```
c_ID = global scalar or vector calculated by a compute with ID
c_ID[I] = Ith component of global vector or Ith column of global array calculated␣
↪by a compute with ID, I can include wildcard (see below)
f_ID = global scalar or vector calculated by a fix with ID
f_ID[I] = Ith component of global vector or Ith column of global array calculated␣
↪by a fix with ID, I can include wildcard (see below)
```

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```
v_name = value(s) calculated by an equal-style or vector-style variable with name
v_name[I] = value calculated by a vector-style variable with name
```

- zero or more keyword/arg pairs may be appended
- keyword = *mode* or *file* or *ave* or *start* or *off* or *overwrite* or *title1* or *title2* or *title3*

```
mode arg = scalar or vector
  scalar = all input values are global scalars
  vector = all input values are global vectors or global arrays
ave args = one or running or window M
  one = output a new average value every Nfreq steps
  running = output cumulative average of all previous Nfreq steps
  window M = output average of M most recent Nfreq steps
start args = Nstart
  Nstart = start averaging on this timestep
off arg = M = do not average this value
  M = value # from 1 to Nvalues
file arg = filename
  filename = name of file to output time averages to
overwrite arg = none = overwrite output file with only latest output
format arg = string
  string = C-style format string
title1 arg = string
  string = text to print as 1st line of output file
title2 arg = string
  string = text to print as 2nd line of output file
title3 arg = string
  string = text to print as 3rd line of output file, only for vector mode
```

16.14.2 Examples

```
fix 1 all ave/time 100 5 1000 c_myTemp c_thermo_temp file temp.profile
fix 1 all ave/time 100 5 1000 c_thermo_press[2] ave window 20 &
                              title1 "My output values"
fix 1 all ave/time 100 5 1000 c_thermo_press[*]
fix 1 all ave/time 1 100 1000 f_indent f_indent[1] file temp.indent off 1
```

16.14.3 Description

Use one or more global values as inputs every few timesteps, and average them over longer timescales. The resulting averages can be used by other *output commands* such as *thermo_style custom*, and can also be written to a file. Note that if no time averaging is done, this command can be used as a convenient way to simply output one or more global values to a file.

The group specified with this command is ignored. However, note that specified values may represent calculations performed by computes and fixes which store their own "group" definitions.

Each listed value can be the result of a *compute* or *fix* or the evaluation of an equal-style or vector-style *variable*. In each case, the compute, fix, or variable must produce a global quantity, not a per-atom or local quantity. If you wish to spatial- or time-average or histogram per-atom quantities from a compute, fix, or variable, then see the *fix ave/chunk*, *fix ave/atom*, or *fix ave/histo* commands. If you wish to sum a per-atom quantity into a single global quantity, see the *compute reduce* command.

Computes that produce global quantities are those which do not have the word *atom* in their style name. Only a few *fixes* produce global quantities. See the doc pages for individual fixes for info on which ones produce such values. *Variables* of style *equal* and *vector* are the only ones that can be used with this fix. Variables of style *atom* cannot be used, since they produce per-atom values.

The input values must either be all scalars or all vectors depending on the setting of the *mode* keyword. In both cases, the averaging is performed independently on each input value. I.e. each input scalar is averaged independently or each element of each input vector is averaged independently.

If *mode* = scalar, then the input values must be scalars, or vectors with a bracketed term appended, indicating the Ith value of the vector is used.

If *mode* = vector, then the input values must be vectors, or arrays with a bracketed term appended, indicating the Ith column of the array is used. All vectors must be the same length, which is the length of the vector or number of rows in the array.

Note that for values from a compute or fix, the bracketed index I can be specified using a wildcard asterisk with the index to effectively specify multiple values. This takes the form "*" or "*n" or "n*" or "m*n". If N = the size of the vector (for *mode* = scalar) or the number of columns in the array (for *mode* = vector), then an asterisk with no numeric values means all indices from 1 to N. A leading asterisk means all indices from 1 to n (inclusive). A trailing asterisk means all indices from n to N (inclusive). A middle asterisk means all indices from m to n (inclusive).

Using a wildcard is the same as if the individual elements of the vector or columns of the array had been listed one by one. E.g. these 2 fix ave/time commands are equivalent, since the *compute rdf* command creates, in this case, a global array with 3 columns, each of length 50:

```
compute myRDF all rdf 50 1 2
fix 1 all ave/time 100 1 100 c_myRDF[*] file tmp1.rdf mode vector
fix 2 all ave/time 100 1 100 c_myRDF[1] c_myRDF[2] c_myRDF[3] file tmp2.rdf␣
↪mode vector
```

The *Nevery*, *Nrepeat*, and *Nfreq* arguments specify on what timesteps the input values will be used in order to contribute to the average. The final averaged quantities are generated on timesteps that are a multiple of *Nfreq*. The average is over *Nrepeat* quantities, computed in the preceding portion of the simulation every *Nevery* timesteps. *Nfreq* must be a multiple of *Nevery* and *Nevery* must be non-zero even if *Nrepeat* is 1. Also, the timesteps contributing to the average value cannot overlap, i.e. Nrepeat*Nevery can not exceed Nfreq.

For example, if Nevery=2, Nrepeat=6, and Nfreq=100, then values on timesteps 90,92,94,96,98,100 will be used to compute the final average on timestep 100. Similarly for timesteps 190,192,194,196,198,200 on timestep 200, etc. If Nrepeat=1 and Nfreq = 100, then no time averaging is done; values are simply generated on timesteps 100,200,etc.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If *mode* = scalar, then if no bracketed term is appended, the global scalar calculated by the compute is used. If a bracketed term is appended, the Ith element of the global vector calculated by the compute is used. If *mode* = vector, then if no bracketed term is appended, the global vector calculated by the compute is used. If a bracketed term is appended, the Ith column of the global array calculated by the compute is used. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

Note that there is a *compute reduce* command which can sum per-atom quantities into a global scalar or vector which can thus be accessed by fix ave/time. Or it can be a compute defined not in your input script, but by *thermodynamic output* or other fixes such as *fix nvt* or *fix temp/rescale*. See the doc pages for these commands which give the IDs of these computes. Users can also write code for their own compute styles and *add them to LAMMPS*.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If *mode* = scalar, then if no bracketed term is appended, the global scalar calculated by the fix is used. If a bracketed term is appended, the Ith element of the global vector calculated by the fix is used. If *mode* = vector, then if no bracketed

term is appended, the global vector calculated by the fix is used. If a bracketed term is appended, the Ith column of the global array calculated by the fix is used. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

Note that some fixes only produce their values on certain timesteps, which must be compatible with *Nevery*, else an error will result. Users can also write code for their own fix styles and *add them to LAMMPS*.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. If *mode* = scalar, then only equal-style or vector-style variables can be used, which both produce global values. In this mode, a vector-style variable requires a bracketed term to specify the Ith element of the vector calculated by the variable. If *mode* = vector, then only a vector-style variable can be used, without a bracketed term. See the *variable* command for details.

Note that variables of style *equal* and *vector* define a formula which can reference individual atom properties or thermodynamic keywords, or they can invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of specifying quantities to time average.

Additional optional keywords also affect the operation of this fix.

If the *mode* keyword is set to *scalar*, then all input values must be global scalars, or elements of global vectors. If the *mode* keyword is set to *vector*, then all input values must be global vectors, or columns of global arrays. They can also be global arrays, which are converted into a series of global vectors (one per column), as explained above.

The *ave* keyword determines how the values produced every *Nfreq* steps are averaged with values produced on previous steps that were multiples of *Nfreq*, before they are accessed by another output command or written to a file.

If the *ave* setting is *one*, then the values produced on timesteps that are multiples of *Nfreq* are independent of each other; they are output as-is without further averaging.

If the *ave* setting is *running*, then the values produced on timesteps that are multiples of *Nfreq* are summed and averaged in a cumulative sense before being output. Each output value is thus the average of the value produced on that timestep with all preceding values. This running average begins when the fix is defined; it can only be restarted by deleting the fix via the *unfix* command, or by re-defining the fix by re-specifying it.

If the *ave* setting is *window*, then the values produced on timesteps that are multiples of *Nfreq* are summed and averaged within a moving "window" of time, so that the last M values are used to produce the output. E.g. if M = 3 and Nfreq = 1000, then the output on step 10000 will be the average of the individual values on steps 8000,9000,10000. Outputs on early steps will average over less than M values if they are not available.

The *start* keyword specifies what timestep averaging will begin on. The default is step 0. Often input values can be 0.0 at time 0, so setting *start* to a larger value can avoid including a 0.0 in a running or windowed average.

The *off* keyword can be used to flag any of the input values. If a value is flagged, it will not be time averaged. Instead the most recent input value will always be stored and output. This is useful if one of more of the inputs produced by a compute or fix or variable are effectively constant or are simply current values. E.g. they are being written to a file with other time-averaged values for purposes of creating well-formatted output.

The *file* keyword allows a filename to be specified. Every *Nfreq* steps, one quantity or vector of quantities is written to the file for each input value specified in the fix ave/time command. For *mode* = scalar, this means a single line is written each time output is performed. Thus the file ends up to be a series of lines, i.e. one column of numbers for each input value. For *mode* = vector, an array of numbers is written each time output is performed. The number of rows is the length of the input vectors, and the number of columns is the number of values. Thus the file ends up to be a series of these array sections.

The *overwrite* keyword will continuously overwrite the output file with the latest output, so that it only contains one timestep worth of output. This option can only be used with the *ave running* setting.

The *format* keyword sets the numeric format of each value when it is printed to a file via the *file* keyword. Note that all values are floating point quantities. The default format is %g. You can specify a higher precision if desired, e.g. %20.16g.

The *title1* and *title2* and *title3* keywords allow specification of the strings that will be printed as the first 2 or 3 lines of the output file, assuming the *file* keyword was used. LAMMPS uses default values for each of these, so they do not need to be specified.

By default, these header lines are as follows for *mode* = scalar:

```
# Time-averaged data for fix ID
# TimeStep value1 value2 ...
```

In the first line, ID is replaced with the fix-ID. In the second line the values are replaced with the appropriate fields from the fix ave/time command. There is no third line in the header of the file, so the *title3* setting is ignored when *mode* = scalar.

By default, these header lines are as follows for *mode* = vector:

```
# Time-averaged data for fix ID
# TimeStep Number-of-rows
# Row value1 value2 ...
```

In the first line, ID is replaced with the fix-ID. The second line describes the two values that are printed at the first of each section of output. In the third line the values are replaced with the appropriate fields from the fix ave/time command.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix produces a global scalar or global vector or global array which can be accessed by various *output commands*. The values can only be accessed on timesteps that are multiples of *Nfreq* since that is when averaging is performed.

A scalar is produced if only a single input value is averaged and *mode* = scalar. A vector is produced if multiple input values are averaged for *mode* = scalar, or a single input value for *mode* = vector. In the first case, the length of the vector is the number of inputs. In the second case, the length of the vector is the same as the length of the input vector. An array is produced if multiple input values are averaged and *mode* = vector. The global array has # of rows = length of the input vectors and # of columns = number of inputs.

If the fix produces a scalar or vector, then the scalar and each element of the vector can be either "intensive" or "extensive", depending on whether the values contributing to the scalar or vector element are "intensive" or "extensive". If the fix produces an array, then all elements in the array must be the same, either "intensive" or "extensive". If a compute or fix provides the value being time averaged, then the compute or fix determines whether the value is intensive or extensive; see the doc page for that compute or fix for further info. Values produced by a variable are treated as intensive.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.14.4 Restrictions

none

16.14.5 Related commands

compute, *fix ave/atom*, *fix ave/chunk*, *fix ave/histo*, *variable*, *fix ave/correlate*,

16.14.6 Default

The option defaults are mode = scalar, ave = one, start = 0, no file output, format = %g, title 1,2,3 = strings as described above, and no off settings for any input values.

16.15 fix aveforce command

16.15.1 Syntax

```
fix ID group-ID aveforce fx fy fz keyword value ...
```

- ID, group-ID are documented in *fix* command
- aveforce = style name of this fix command
- fx,fy,fz = force component values (force units)

  ```
  any of fx,fy,fz can be a variable (see below)
  ```

- zero or more keyword/value pairs may be appended to args
- keyword = *region*

  ```
  region value = region-ID
    region-ID = ID of region atoms must be in to have added force
  ```

16.15.2 Examples

```
fix pressdown topwall aveforce 0.0 -1.0 0.0
fix 2 bottomwall aveforce NULL -1.0 0.0 region top
fix 2 bottomwall aveforce NULL -1.0 v_oscillate region top
```

16.15.3 Description

Apply an additional external force to a group of atoms in such a way that every atom experiences the same force. This is useful for pushing on wall or boundary atoms so that the structure of the wall does not change over time.

The existing force is averaged for the group of atoms, component by component. The actual force on each atom is then set to the average value plus the component specified in this command. This means each atom in the group receives the same force.

Any of the fx,fy,fz values can be specified as NULL which means the force in that dimension is not changed. Note that this is not the same as specifying a 0.0 value, since that sets all forces to the same average value without adding in any additional force.

Any of the 3 quantities defining the force components can be specified as an equal-style *variable*, namely *fx*, *fy*, *fz*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the average force.

Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent average force.

If the *region* keyword is used, the atom must also be in the specified geometric *region* in order to have force added to it.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify* *respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix is adding its forces. Default is the outermost level.

This fix computes a global 3-vector of forces, which can be accessed by various *output commands*. This is the total force on the group of atoms before the forces on individual atoms are changed by the fix. The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command. You should not specify force components with a variable that has time-dependence for use with a minimizer, since the minimizer increments the timestep as the iteration count during the minimization.

16.15.4 Restrictions

none

16.15.5 Related commands

fix setforce, *fix addforce*

Default: none

16.16 fix balance command

16.16.1 Syntax

```
fix ID group-ID balance Nfreq thresh style args keyword args ...
```

- ID, group-ID are documented in *fix* command
- balance = style name of this fix command
- Nfreq = perform dynamic load balancing every this many steps
- thresh = imbalance threshold that must be exceeded to perform a re-balance
- style = *shift* or *rcb*

```
shift args = dimstr Niter stopthresh
  dimstr = sequence of letters containing "x" or "y" or "z", each not␣
↪more than once
  Niter = # of times to iterate within each dimension of dimstr sequence
  stopthresh = stop balancing when this imbalance threshold is reached
rcb args = none
```

- zero or more keyword/arg pairs may be appended
- keyword = *weight* or *out*

```
weight style args = use weighted particle counts for the balancing
  style = group or neigh or time or var or store
    group args = Ngroup group1 weight1 group2 weight2 ...
      Ngroup = number of groups with assigned weights
      group1, group2, ... = group IDs
      weight1, weight2, ...   = corresponding weight factors
    neigh factor = compute weight based on number of neighbors
      factor = scaling factor (> 0)
    time factor = compute weight based on time spend computing
      factor = scaling factor (> 0)
    var name = take weight from atom-style variable
      name = name of the atom-style variable
    store name = store weight in custom atom property defined by fix␣
↪property/atom command
      name = atom property name (without d_ prefix)
out arg = filename
  filename = write each processor's sub-domain to a file, at each␣
↪re-balancing
```

16.16.2 Examples

```
fix 2 all balance 1000 1.05 shift x 10 1.05
fix 2 all balance 100 0.9 shift xy 20 1.1 out tmp.balance
fix 2 all balance 100 0.9 shift xy 20 1.1 weight group 3 substrate 3.0 solvent 1.0␣
↪solute 0.8 out tmp.balance
fix 2 all balance 100 1.0 shift x 10 1.1 weight time 0.8
fix 2 all balance 100 1.0 shift xy 5 1.1 weight var myweight weight neigh 0.6 weight␣
↪store allweight
fix 2 all balance 1000 1.1 rcb
```

16.16.3 Description

This command adjusts the size and shape of processor sub-domains within the simulation box, to attempt to balance the number of particles and thus the computational cost (load) evenly across processors. The load balancing is "dynamic" in the sense that re-balancing is performed periodically during the simulation. To perform "static" balancing, before or between runs, see the *balance* command.

Load-balancing is typically most useful if the particles in the simulation box have a spatially-varying density distribution or where the computational cost varies significantly between different atoms. E.g. a model of a vapor/liquid interface, or a solid with an irregular-shaped geometry containing void regions, or *hybrid pair style simulations* which combine pair styles with different computational cost. In these cases, the LAMMPS default of dividing the simulation box volume into a regular-spaced grid of 3d bricks, with one equal-volume sub-domain per processor, may assign numbers of particles per processor in a way that the computational effort varies significantly. This can lead to poor performance when the simulation is run in parallel.

The balancing can be performed with or without per-particle weighting. With no weighting, the balancing attempts to assign an equal number of particles to each processor. With weighting, the balancing attempts to assign an equal aggregate computational weight to each processor, which typically induces a different number of atoms assigned to each processor.

Note: The weighting options listed above are documented with the *balance* command in *this section of the balance command* doc page. That section describes the various weighting options and gives a few examples of how they can be used. The weighting options are the same for both the fix balance and *balance* commands.

Note that the *processors* command allows some control over how the box volume is split across processors. Specifically, for a Px by Py by Pz grid of processors, it allows choice of Px, Py, and Pz, subject to the constraint that Px * Py * Pz = P, the total number of processors. This is sufficient to achieve good load-balance for some problems on some processor counts. However, all the processor sub-domains will still have the same shape and same volume.

On a particular timestep, a load-balancing operation is only performed if the current "imbalance factor" in particles owned by each processor exceeds the specified *thresh* parameter. The imbalance factor is defined as the maximum number of particles (or weight) owned by any processor, divided by the average number of particles (or weight) per processor. Thus an imbalance factor of 1.0 is perfect balance.

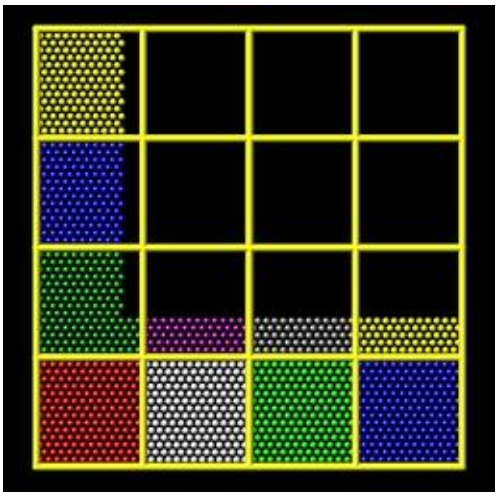
As an example, for 10000 particles running on 10 processors, if the most heavily loaded processor has 1200 particles, then the factor is 1.2, meaning there is a 20% imbalance. Note that re-balances can be forced even if the current balance is perfect (1.0) be specifying a *thresh* < 1.0.

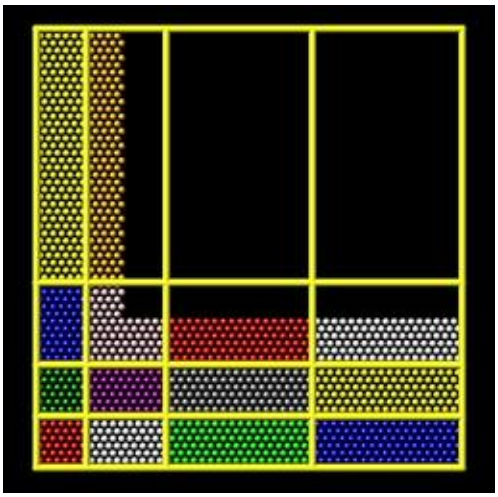
Note: This command attempts to minimize the imbalance factor, as defined above. But depending on the method a perfect balance (1.0) may not be achieved. For example, "grid" methods (defined below) that create a logical 3d grid cannot achieve perfect balance for many irregular distributions of particles. Likewise, if a portion of the system is a perfect lattice, e.g. the initial system is generated by the *create_atoms* command, then "grid" methods may be unable to achieve exact balance. This is because entire lattice planes will be owned or not owned by a single processor.

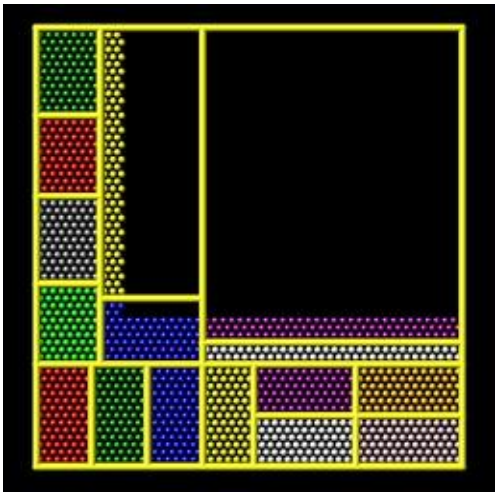
Note: The imbalance factor is also an estimate of the maximum speed-up you can hope to achieve by running a perfectly balanced simulation versus an imbalanced one. In the example above, the 10000 particle simulation could run up to 20% faster if it were perfectly balanced, versus when imbalanced. However, computational cost is not strictly proportional to particle count, and changing the relative size and shape of processor sub-domains may lead to additional computational and communication overheads, e.g. in the PPPM solver used via the *kspace_style* command. Thus you should benchmark the run times of a simulation before and after balancing.

The method used to perform a load balance is specified by one of the listed styles, which are described in detail below. There are 2 kinds of styles.

The *shift* style is a "grid" method which produces a logical 3d grid of processors. It operates by changing the cutting planes (or lines) between processors in 3d (or 2d), to adjust the volume (area in 2d) assigned to each processor, as in the following 2d diagram where processor sub-domains are shown and atoms are colored by the processor that owns them. The leftmost diagram is the default partitioning of the simulation box across processors (one sub-box for each of 16 processors); the middle diagram is after a "grid" method has been applied.







The *rcb* style is a "tiling" method which does not produce a logical 3d grid of processors. Rather it tiles the simulation domain with rectangular sub-boxes of varying size and shape in an irregular fashion so as to have equal numbers of particles (or weight) in each sub-box, as in the rightmost diagram above.

The "grid" methods can be used with either of the *comm_style* command options, *brick* or *tiled*. The "tiling" methods can only be used with *comm_style tiled*.

When a "grid" method is specified, the current domain partitioning can be either a logical 3d grid or a tiled partitioning. In the former case, the current logical 3d grid is used as a starting point and changes are made to improve the imbalance factor. In the latter case, the tiled partitioning is discarded and a logical 3d grid is created with uniform spacing in all dimensions. This is the starting point for the balancing operation.

When a "tiling" method is specified, the current domain partitioning ("grid" or "tiled") is ignored, and a new partitioning is computed from scratch.

The *group-ID* is ignored. However the impact of balancing on different groups of atoms can be affected by using the *group* weight style as described below.

The *Nfreq* setting determines how often a re-balance is performed. If *Nfreq* > 0, then re-balancing will occur every *Nfreq* steps. Each time a re-balance occurs, a reneighboring is triggered, so *Nfreq* should not be too small. If *Nfreq* = 0, then re-balancing will be done every time reneighboring normally occurs, as determined by the the *neighbor* and *neigh_modify* command settings.

On re-balance steps, re-balancing will only be attempted if the current imbalance factor, as defined above, exceeds the *thresh* setting.

The *shift* style invokes a "grid" method for balancing, as described above. It changes the positions of cutting planes between processors in an iterative fashion, seeking to reduce the imbalance factor.

The *dimstr* argument is a string of characters, each of which must be an "x" or "y" or "z". Eacn character can appear zero or one time, since there is no advantage to balancing on a dimension more than once. You should normally only list dimensions where you expect there to be a density variation in the particles.

Balancing proceeds by adjusting the cutting planes in each of the dimensions listed in *dimstr*, one dimension at a time. For a single dimension, the balancing operation (described below) is iterated on up to *Niter* times. After each dimension finishes, the imbalance factor is re-computed, and the balancing operation halts if the *stopthresh* criterion is met.

A re-balance operation in a single dimension is performed using a density-dependent recursive multisectioning algorithm, where the position of each cutting plane (line in 2d) in the dimension is adjusted independently. This is similar

to a recursive bisectioning for a single value, except that the bounds used for each bisectioning take advantage of information from neighboring cuts if possible, as well as counts of particles at the bounds on either side of each cuts, which themselves were cuts in previous iterations. The latter is used to infer a density of particles near each of the current cuts. At each iteration, the count of particles on either side of each plane is tallied. If the counts do not match the target value for the plane, the position of the cut is adjusted based on the local density. The low and high bounds are adjusted on each iteration, using new count information, so that they become closer together over time. Thus as the recursion progresses, the count of particles on either side of the plane gets closer to the target value.

The density-dependent part of this algorithm is often an advantage when you re-balance a system that is already nearly balanced. It typically converges more quickly than the geometric bisectioning algorithm used by the *balance* command. However, if can be a disadvantage if you attempt to re-balance a system that is far from balanced, and converge more slowly. In this case you probably want to use the *balance* command before starting a run, so that you begin the run with a balanced system.

Once the re-balancing is complete and final processor sub-domains assigned, particles migrate to their new owning processor as part of the normal reneighboring procedure.

Note: At each re-balance operation, the bisectioning for each cutting plane (line in 2d) typically starts with low and high bounds separated by the extent of a processor's sub-domain in one dimension. The size of this bracketing region shrinks based on the local density, as described above, which should typically be 1/2 or more every iteration. Thus if *Niter* is specified as 10, the cutting plane will typically be positioned to better than 1 part in 1000 accuracy (relative to the perfect target position). For *Niter* = 20, it will be accurate to better than 1 part in a million. Thus there is no need to set *Niter* to a large value. This is especially true if you are re-balancing often enough that each time you expect only an incremental adjustment in the cutting planes is necessary. LAMMPS will check if the threshold accuracy is reached (in a dimension) is less iterations than *Niter* and exit early.

The *rcb* style invokes a "tiled" method for balancing, as described above. It performs a recursive coordinate bisectioning (RCB) of the simulation domain. The basic idea is as follows.

The simulation domain is cut into 2 boxes by an axis-aligned cut in the longest dimension, leaving one new box on either side of the cut. All the processors are also partitioned into 2 groups, half assigned to the box on the lower side of the cut, and half to the box on the upper side. (If the processor count is odd, one side gets an extra processor.) The cut is positioned so that the number of atoms in the lower box is exactly the number that the processors assigned to that box should own for load balance to be perfect. This also makes load balance for the upper box perfect. The positioning is done iteratively, by a bisectioning method. Note that counting atoms on either side of the cut requires communication between all processors at each iteration.

That is the procedure for the first cut. Subsequent cuts are made recursively, in exactly the same manner. The subset of processors assigned to each box make a new cut in the longest dimension of that box, splitting the box, the subset of processors, and the atoms in the box in two. The recursion continues until every processor is assigned a sub-box of the entire simulation domain, and owns the atoms in that sub-box.

The *out* keyword writes text to the specified *filename* with the results of each re-balancing operation. The file contains the bounds of the sub-domain for each processor after the balancing operation completes. The format of the file is compatible with the Pizza.py *mdump* tool which has support for manipulating and visualizing mesh files. An example is shown here for a balancing by 4 processors for a 2d problem:

```
ITEM: TIMESTEP
0
ITEM: NUMBER OF NODES
16
ITEM: BOX BOUNDS
```

(continues on next page)

(continued from previous page)

```
0 10
0 10
0 10
ITEM: NODES
1 1 0 0 0
2 1 5 0 0
3 1 5 5 0
4 1 0 5 0
5 1 5 0 0
6 1 10 0 0
7 1 10 5 0
8 1 5 5 0
9 1 0 5 0
10 1 5 5 0
11 1 5 10 0
12 1 10 5 0
13 1 5 5 0
14 1 10 5 0
15 1 10 10 0
16 1 5 10 0
ITEM: TIMESTEP
0
ITEM: NUMBER OF SQUARES
4
ITEM: SQUARES
1 1 1 2 3 4
2 1 5 6 7 8
3 1 9 10 11 12
4 1 13 14 15 16
```

The coordinates of all the vertices are listed in the NODES section, 5 per processor. Note that the 4 sub-domains share vertices, so there will be duplicate nodes in the list.

The "SQUARES" section lists the node IDs of the 4 vertices in a rectangle for each processor (1 to 4).

For a 3d problem, the syntax is similar with 8 vertices listed for each processor, instead of 4, and "SQUARES" replaced by "CUBES".

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix computes a global scalar which is the imbalance factor after the most recent re-balance and a global vector of length 3 with additional information about the most recent re-balancing. The 3 values in the vector are as follows:

- 1 = max # of particles per processor
- 2 = total # iterations performed in last re-balance
- 3 = imbalance factor right before the last re-balance was performed

As explained above, the imbalance factor is the ratio of the maximum number of particles (or total weight) on any processor to the average number of particles (or total weight) per processor.

These quantities can be accessed by various *output commands*. The scalar and vector values calculated by this fix are "intensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.16.4 Restrictions

For 2d simulations, the *z* style cannot be used. Nor can a "z" appear in *dimstr* for the *shift* style.

Balancing through recursive bisectioning (*rcb* style) requires *comm_style tiled*

16.16.5 Related commands

group, *processors*, *balance*, *comm_style*

Default: none

16.17 fix bocs command

16.17.1 Syntax

```
fix  ID group-ID bocs keyword values ...

keyword = temp or cgiso or analytic or linear_spline or cubic_spline
  temp values = Tstart Tstop Tdamp
  cgiso values = Pstart Pstop Pdamp
  basis set
    analytic values = V_avg N_particles N_coeff Coeff_1 Coeff_2 ... Coeff_N
    linear_spline values = input_filename
    cubic_spline values = input_filename
```

16.17.2 Examples

```
fix 1 all bocs temp 300.0 300.0 100.0 cgiso 0.986 0.986 1000.0 analytic 66476.015 968␣
↪2 245030.10 8962.20

fix 1 all bocs temp 300.0 300.0 100.0 cgiso 0.986 0.986 1000.0 cubic_spline input_Fv.
↪dat

thermo_modify press 1_press
```

16.17.3 Description

These commands incorporate a pressure correction as described by Dunn and Noid in *(Dunn1)* to the standard MTTK barostat by Martyna et. al. in *(Martyna)* . The first half of the command mimics a standard fix npt command:

```
fix 1 all bocs temp Tstart Tstop Tcoupl cgiso Pstart Pstop Pdamp
```

The two differences are replacing *npt* with *bocs*, and replacing *iso*/*aniso*/*etc* with *cgiso*. The rest of the command details what form you would like to use for the pressure correction equation. The choices are: *analytic*, *linear_spline*, or *cubic_spline*.

With either spline method, the only argument that needs to follow it is the name of a file that contains the desired pressure correction as a function of volume. The file must be formatted so each line has:

```
Volume_i, PressureCorrection_i
```

Note both the COMMA and the SPACE separating the volume's value and its corresponding pressure correction. The volumes in the file must be uniformly spaced. Both the volumes and the pressure corrections should be provided in the proper units, e.g. if you are using *units real*, the volumes should all be in cubic angstroms, and the pressure corrections should all be in atmospheres. Furthermore, the table should start/end at a volume considerably smaller/larger than you expect your system to sample during the simulation. If the system ever reaches a volume outside of the range provided, the simulation will stop.

With the *analytic* option, the arguments are as follows:

```
... analytic V_avg N_particles N_coeff Coeff_1 Coeff_2 ... Coeff_N
```

Note that *V_avg* and *Coeff_i* should all be in the proper units, e.g. if you are using *units real*, *V_avg* should be in cubic angstroms, and the coefficients should all be in atmospheres * cubic angstroms.

16.17.4 Restrictions

As this is computing a (modified) pressure, group-ID should be *all*.

The pressure correction has only been tested for use with an isotropic pressure coupling in 3 dimensions.

By default, LAMMPS will still report the normal value for the pressure if the pressure is printed via a *thermo* command, or if the pressures are written to a file every so often. In order to have LAMMPS report the modified pressure, you must include the *thermo_modify* command given in the examples. For the last argument in the command, you should put XXXX_press, where XXXX is the ID given to the fix bocs command (in the example, the ID of the fix bocs command is 1).

This fix is part of the USER-BOCS package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Related:

For more details about the pressure correction and the entire BOCS software package, visit the BOCS package on GitHub and read the release paper by Dunn et. al. *(Dunn2)* .

(Dunn1) Dunn and Noid, J Chem Phys, 143, 243148 (2015).

(Martyna) Martyna, Tobias, and Klein, J Chem Phys, 101, 4177 (1994).

(Dunn2) Dunn, Lebold, DeLyser, Rudzinski, and Noid, J. Phys. Chem. B, 122, 3363 (2018).

16.18 fix bond/break command

16.18.1 Syntax

```
fix ID group-ID bond/break Nevery bondtype Rmax keyword values ...
```

- ID, group-ID are documented in *fix* command
- bond/break = style name of this fix command

- Nevery = attempt bond breaking every this many steps
- bondtype = type of bonds to break
- Rmax = bond longer than Rmax can break (distance units)
- zero or more keyword/value pairs may be appended to args
- keyword = *prob*

```
prob values = fraction seed
  fraction = break a bond with this probability if otherwise eligible
  seed = random number seed (positive integer)
```

16.18.2 Examples

```
fix 5 all bond/break 10 2 1.2
fix 5 polymer bond/break 1 1 2.0 prob 0.5 49829
```

16.18.3 Description

Break bonds between pairs of atoms as a simulation runs according to specified criteria. This can be used to model the dissolution of a polymer network due to stretching of the simulation box or other deformations. In this context, a bond means an interaction between a pair of atoms computed by the *bond_style* command. Once the bond is broken it will be permanently deleted, as will all angle, dihedral, and improper interactions that bond is part of.

This is different than a *pairwise* bond-order potential such as Tersoff or AIREBO which infers bonds and many-body interactions based on the current geometry of a small cluster of atoms and effectively creates and destroys bonds and higher-order many-body interactions from timestep to timestep as atoms move.

A check for possible bond breakage is performed every *Nevery* timesteps. If two bonded atoms I,J are further than a distance *Rmax* of each other, if the bond is of type *bondtype*, and if both I and J are in the specified fix group, then I,J is labeled as a "possible" bond to break.

If several bonds involving an atom are stretched, it may have multiple possible bonds to break. Every atom checks its list of possible bonds to break and labels the longest such bond as its "sole" bond to break. After this is done, if atom I is bonded to atom J in its sole bond, and atom J is bonded to atom I in its sole bond, then the I,J bond is "eligible" to be broken.

Note that these rules mean an atom will only be part of at most one broken bond on a given timestep. It also means that if atom I chooses atom J as its sole partner, but atom J chooses atom K is its sole partner (due to Rjk > Rij), then this means atom I will not be part of a broken bond on this timestep, even if it has other possible bond partners.

The *prob* keyword can effect whether an eligible bond is actually broken. The *fraction* setting must be a value between 0.0 and 1.0. A uniform random number between 0.0 and 1.0 is generated and the eligible bond is only broken if the random number < fraction.

When a bond is broken, data structures within LAMMPS that store bond topology are updated to reflect the breakage. Likewise, if the bond is part of a 3-body (angle) or 4-body (dihedral, improper) interaction, that interaction is removed as well. These changes typically affect pairwise interactions between atoms that used to be part of bonds, angles, etc.

Note: One data structure that is not updated when a bond breaks are the molecule IDs stored by each atom. Even though one molecule becomes two molecules due to the broken bond, all atoms in both new molecules retain their original molecule IDs.

Computationally, each timestep this fix operates, it loops over all the bonds in the system and computes distances between pairs of bonded atoms. It also communicates between neighboring processors to coordinate which bonds are broken. Moreover, if any bonds are broken, neighbor lists must be immediately updated on the same timestep. This is to insure that any pairwise interactions that should be turned "on" due to a bond breaking, because they are no longer excluded by the presence of the bond and the settings of the *special_bonds* command, will be immediately recognized. All of these operations increase the cost of a timestep. Thus you should be cautious about invoking this fix too frequently.

You can dump out snapshots of the current bond topology via the *dump local* command.

Note: Breaking a bond typically alters the energy of a system. You should be careful not to choose bond breaking criteria that induce a dramatic change in energy. For example, if you define a very stiff harmonic bond and break it when 2 atoms are separated by a distance far from the equilibrium bond length, then the 2 atoms will be dramatically released when the bond is broken. More generally, you may need to thermostat your system to compensate for energy changes resulting from broken bonds (and angles, dihedrals, impropers).

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix computes two statistics which it stores in a global vector of length 2, which can be accessed by various *output commands*. The vector values calculated by this fix are "intensive".

These are the 2 quantities:

- (1) # of bonds broken on the most recent breakage timestep
- (2) cumulative # of bonds broken

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.18.4 Restrictions

This fix is part of the MC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.18.5 Related commands

fix bond/create, *fix bond/react*, *fix bond/swap*, *dump local*, *special_bonds*

16.18.6 Default

The option defaults are prob = 1.0.

16.19 fix bond/create command

16.19.1 Syntax

```
fix ID group-ID bond/create Nevery itype jtype Rmin bondtype keyword values ...
```

- ID, group-ID are documented in *fix* command
- bond/create = style name of this fix command
- Nevery = attempt bond creation every this many steps
- itype,jtype = atoms of itype can bond to atoms of jtype
- Rmin = 2 atoms separated by less than Rmin can bond (distance units)
- bondtype = type of created bonds
- zero or more keyword/value pairs may be appended to args
- keyword = *iparam* or *jparam* or *prob* or *atype* or *dtype* or *itype*

```
iparam values = maxbond, newtype
  maxbond = max # of bonds of bondtype the itype atom can have
  newtype = change the itype atom to this type when maxbonds exist
jparam values = maxbond, newtype
  maxbond = max # of bonds of bondtype the jtype atom can have
  newtype = change the jtype atom to this type when maxbonds exist
prob values = fraction seed
  fraction = create a bond with this probability if otherwise eligible
  seed = random number seed (positive integer)
atype value = angletype
  angletype = type of created angles
dtype value = dihedraltype
  dihedraltype = type of created dihedrals
itype value = impropertype
  impropertype = type of created impropers
```

16.19.2 Examples

```
fix 5 all bond/create 10 1 2 0.8 1
fix 5 all bond/create 1 3 3 0.8 1 prob 0.5 85784 iparam 2 3
fix 5 all bond/create 1 3 3 0.8 1 prob 0.5 85784 iparam 2 3 atype 1 dtype 2
```

16.19.3 Description

Create bonds between pairs of atoms as a simulation runs according to specified criteria. This can be used to model cross-linking of polymers, the formation of a percolation network, etc. In this context, a bond means an interaction between a pair of atoms computed by the *bond_style* command. Once the bond is created it will be permanently in place. Optionally, the creation of a bond can also create angle, dihedral, and improper interactions that bond is part of. See the discussion of the *atype*, *dtype*, and *itype* keywords below.

This is different than a *pairwise* bond-order potential such as Tersoff or AIREBO which infers bonds and many-body interactions based on the current geometry of a small cluster of atoms and effectively creates and destroys bonds and higher-order many-body interactions from timestep to timestep as atoms move.

A check for possible new bonds is performed every *Nevery* timesteps. If two atoms I,J are within a distance *Rmin* of each other, if I is of atom type *itype*, if J is of atom type *jtype*, if both I and J are in the specified fix group, if a bond does not already exist between I and J, and if both I and J meet their respective *maxbond* requirement (explained below), then I,J is labeled as a "possible" bond pair.

If several atoms are close to an atom, it may have multiple possible bond partners. Every atom checks its list of possible bond partners and labels the closest such partner as its "sole" bond partner. After this is done, if atom I has atom J as its sole partner, and atom J has atom I as its sole partner, then the I,J bond is "eligible" to be formed.

Note that these rules mean an atom will only be part of at most one created bond on a given timestep. It also means that if atom I chooses atom J as its sole partner, but atom J chooses atom K is its sole partner (due to Rjk < Rij), then this means atom I will not form a bond on this timestep, even if it has other possible bond partners.

It is permissible to have *itype* = *jtype*. *Rmin* must be <= the pairwise cutoff distance between *itype* and *jtype* atoms, as defined by the *pair_style* command.

The *iparam* and *jparam* keywords can be used to limit the bonding functionality of the participating atoms. Each atom keeps track of how many bonds of *bondtype* it already has. If atom I of itype already has *maxbond* bonds (as set by the *iparam* keyword), then it will not form any more. Likewise for atom J. If *maxbond* is set to 0, then there is no limit on the number of bonds that can be formed with that atom.

The *newtype* value for *iparam* and *jparam* can be used to change the atom type of atom I or J when it reaches *maxbond* number of bonds of type *bondtype*. This means it can now interact in a pairwise fashion with other atoms in a different way by specifying different *pair_coeff* coefficients. If you do not wish the atom type to change, simply specify *newtype* as *itype* or *jtype*.

The *prob* keyword can also effect whether an eligible bond is actually created. The *fraction* setting must be a value between 0.0 and 1.0. A uniform random number between 0.0 and 1.0 is generated and the eligible bond is only created if the random number < fraction.

Any bond that is created is assigned a bond type of *bondtype*

When a bond is created, data structures within LAMMPS that store bond topology are updated to reflect the creation. If the bond is part of new 3-body (angle) or 4-body (dihedral, improper) interactions, you can choose to create new angles, dihedrals, impropers as well, using the *atype*, *dtype*, and *itype* keywords. All of these changes typically affect pairwise interactions between atoms that are now part of new bonds, angles, etc.

Note: One data structure that is not updated when a bond breaks are the molecule IDs stored by each atom. Even though two molecules become one molecule due to the created bond, all atoms in the new molecule retain their original molecule IDs.

If the *atype* keyword is used and if an angle potential is defined via the *angle_style* command, then any new 3-body interactions inferred by the creation of a bond will create new angles of type *angletype*, with parameters assigned by the corresponding *angle_coeff* command. Likewise, the *dtype* and *itype* keywords will create new dihedrals and impropers of type *dihedraltype* and *impropertype*.

Note: To create a new bond, the internal LAMMPS data structures that store this information must have space for it. When LAMMPS is initialized from a data file, the list of bonds is scanned and the maximum number of bonds per atom is tallied. If some atom will acquire more bonds than this limit as this fix operates, then the "extra bond per atom" parameter must be set to allow for it. Ditto for "extra angle per atom", "extra dihedral per atom", and "extra improper per atom" if angles, dihedrals, or impropers are being added when bonds are created. See the *read_data* or *create_box* command for more details. Note that a data file with no atoms can be used if you wish to add non-bonded atoms via the *create atoms* command, e.g. for a percolation simulation.

Note: LAMMPS stores and maintains a data structure with a list of the 1st, 2nd, and 3rd neighbors of each atom

(within the bond topology of the system) for use in weighting pairwise interactions for bonded atoms. Note that adding a single bond always adds a new 1st neighbor but may also induce *many* new 2nd and 3rd neighbors, depending on the molecular topology of your system. The "extra special per atom" parameter must typically be set to allow for the new maximum total size (1st + 2nd + 3rd neighbors) of this per-atom list. There are 2 ways to do this. See the *read_data* or *create_box* commands for details.

Note: Even if you do not use the *atype*, *dtype*, or *itype* keywords, the list of topological neighbors is updated for atoms affected by the new bond. This in turn affects which neighbors are considered for pairwise interactions, using the weighting rules set by the *special_bonds* command. Consider a new bond created between atoms I,J. If J has a bonded neighbor K, then K becomes a 2nd neighbor of I. Even if the *atype* keyword is not used to create angle I-J-K, the pairwise interaction between I and K will be potentially turned off or weighted by the 1-3 weighting specified by the *special_bonds* command. This is the case even if the "angle yes" option was used with that command. The same is true for 3rd neighbors (1-4 interactions), the *dtype* keyword, and the "dihedral yes" option used with the *special_bonds* command.

Note that even if your simulation starts with no bonds, you must define a *bond_style* and use the *bond_coeff* command to specify coefficients for the *bondtype*. Similarly, if new atom types are specified by the *iparam* or *jparam* keywords, they must be within the range of atom types allowed by the simulation and pairwise coefficients must be specified for the new types.

Computationally, each timestep this fix operates, it loops over neighbor lists and computes distances between pairs of atoms in the list. It also communicates between neighboring processors to coordinate which bonds are created. Moreover, if any bonds are created, neighbor lists must be immediately updated on the same timestep. This is to insure that any pairwise interactions that should be turned "off" due to a bond creation, because they are now excluded by the presence of the bond and the settings of the *special_bonds* command, will be immediately recognized. All of these operations increase the cost of a timestep. Thus you should be cautious about invoking this fix too frequently.

You can dump out snapshots of the current bond topology via the *dump local* command.

Note: Creating a bond typically alters the energy of a system. You should be careful not to choose bond creation criteria that induce a dramatic change in energy. For example, if you define a very stiff harmonic bond and create it when 2 atoms are separated by a distance far from the equilibrium bond length, then the 2 atoms will oscillate dramatically when the bond is formed. More generally, you may need to thermostat your system to compensate for energy changes resulting from created bonds (and angles, dihedrals, impropers).

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix computes two statistics which it stores in a global vector of length 2, which can be accessed by various *output commands*. The vector values calculated by this fix are "intensive".

These are the 2 quantities:

- (1) # of bonds created on the most recent creation timestep
- (2) cumulative # of bonds created

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.19.4 Restrictions

This fix is part of the MC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.19.5 Related commands

fix bond/break, *fix bond/react*, *fix bond/swap*, *dump local*, *special_bonds*

16.19.6 Default

The option defaults are iparam = (0,itype), jparam = (0,jtype), and prob = 1.0.

16.20 fix bond/react command

16.20.1 Syntax

```
fix ID group-ID bond/react common_keyword values ...
  react react-ID react-group-ID Nevery Rmin Rmax template-ID(pre-reacted) template-
↪ID(post-reacted) map_file individual_keyword values ...
  react react-ID react-group-ID Nevery Rmin Rmax template-ID(pre-reacted) template-
↪ID(post-reacted) map_file individual_keyword values ...
  react react-ID react-group-ID Nevery Rmin Rmax template-ID(pre-reacted) template-
↪ID(post-reacted) map_file individual_keyword values ...
  ...
```

- ID, group-ID are documented in *fix* command. Group-ID is ignored.
- bond/react = style name of this fix command
- the common keyword/values may be appended directly after 'bond/react'
- this applies to all reaction specifications (below)
- common_keyword = *stabilization*

```
stabilization values = no or yes group-ID xmax
  no = no reaction site stabilization
  yes = perform reaction site stabilization
    group-ID = user-assigned prefix for the dynamic group of atoms not␣
↪currently involved in a reaction
    xmax = xmax value that is used by an internally-created nve/limit␣
↪integrator
```

- react = mandatory argument indicating new reaction specification
- react-ID = user-assigned name for the reaction
- react-group-ID = only atoms in this group are considered for the reaction
- Nevery = attempt reaction every this many steps
- Rmin = bonding pair atoms must be separated by more than Rmin to initiate reaction (distance units)
- Rmax = bonding pair atoms must be separated by less than Rmax to initiate reaction (distance units)
- template-ID(pre-reacted) = ID of a molecule template containing pre-reaction topology

- template-ID(post-reacted) = ID of a molecule template containing post-reaction topology
- map_file = name of file specifying corresponding atom-IDs in the pre- and post-reacted templates
- zero or more individual keyword/value pairs may be appended to each react argument
- individual_keyword = *prob* or *max_rxn* or *stabilize_steps* or *update_edges*

```
prob values = fraction seed
  fraction = initiate reaction with this probability if otherwise eligible
  seed = random number seed (positive integer)
max_rxn value = N
  N = maximum number of reactions allowed to occur
stabilize_steps value = timesteps
  timesteps = number of timesteps to apply the internally-created nve/
↪limit fix to reacting atoms
update_edges value = none or charges or custom
  none = do not update topology near the edges of reaction templates
  charges = update atomic charges of all atoms in reaction templates
  custom = force the update of user-specified atomic charges
```

16.20.2 Examples

For unabridged example scripts and files, see examples/USER/misc/bond_react.

```
molecule mol1 pre_reacted_topology.txt
molecule mol2 post_reacted_topology.txt
fix 5 all bond/react react myrxn1 all 1 0 3.25 mol1 mol2 map_file.txt

molecule mol1 pre_reacted_rxn1.txt
molecule mol2 post_reacted_rxn1.txt
molecule mol3 pre_reacted_rxn2.txt
molecule mol4 post_reacted_rxn2.txt
fix 5 all bond/react stabilization yes nvt_grp .03 &
  react myrxn1 all 1 0 3.25 mol1 mol2 map_file_rxn1.txt prob 0.50 12345 &
  react myrxn2 all 1 0 2.75 mol3 mol4 map_file_rxn2.txt prob 0.25 12345
fix 6 nvt_grp_REACT nvt temp 300 300 100 # set thermostat after bond/react
```

16.20.3 Description

Initiate complex covalent bonding (topology) changes. These topology changes will be referred to as 'reactions' throughout this documentation. Topology changes are defined in pre- and post-reaction molecule templates and can include creation and deletion of bonds, angles, dihedrals, impropers, bond types, angle types, dihedral types, atom types, or atomic charges. In addition, reaction by-products or other molecules can be identified and deleted.

Fix bond/react does not use quantum mechanical (eg. fix qmmm) or pairwise bond-order potential (eg. Tersoff or AIREBO) methods to determine bonding changes a priori. Rather, it uses a distance-based probabilistic criteria to effect predetermined topology changes in simulations using standard force fields.

This fix was created to facilitate the dynamic creation of polymeric, amorphous or highly cross-linked systems. A suggested workflow for using this fix is: 1) identify a reaction to be simulated 2) build a molecule template of the reaction site before the reaction has occurred 3) build a molecule template of the reaction site after the reaction has occurred 4) create a map that relates the template-atom-IDs of each atom between pre- and post-reaction molecule templates 5) fill a simulation box with molecules and run a simulation with fix bond/react.

Only one 'fix bond/react' command can be used at a time. Multiple reactions can be simultaneously applied by specifying multiple *react* arguments to a single 'fix bond/react' command. This syntax is necessary because the 'common keywords' are applied to all reactions.

The *stabilization* keyword enables reaction site stabilization. Reaction site stabilization is performed by including reacting atoms in an internally-created fix *nve/limit* time integrator for a set number of timesteps given by the *stabilize_steps* keyword. While reacting atoms are being time integrated by the internal nve/limit, they are prevented from being involved in any new reactions. The *xmax* value keyword should typically be set to the maximum distance that non-reacting atoms move during the simulation.

Fix bond/react creates and maintains two important dynamic groups of atoms when using the *stabilization* keyword. The first group contains all atoms currently involved in a reaction; this group is automatically thermostatted by an internally-created *nve/limit* integrator. The second group contains all atoms currently not involved in a reaction. This group should be used by a thermostat in order to time integrate the system. The name of this group of non-reacting atoms is created by appending '_REACT' to the group-ID argument of the *stabilization* keyword, as shown in the second example above.

Note: When using reaction stabilization, you should generally not have a separate thermostat which acts on the 'all' group.

The group-ID set using the *stabilization* keyword can be an existing static group or a previously-unused group-ID. It cannot be specified as 'all'. If the group-ID is previously unused, the fix bond/react command creates a *dynamic group* that is initialized to include all atoms. If the group-ID is that of an existing static group, the group is used as the parent group of new, internally-created dynamic group. In both cases, this new dynamic group is named by appending '_REACT' to the group-ID, e.g. nvt_grp_REACT. By specifying an existing group, you may thermostat constant-topology parts of your system separately. The dynamic group contains only atoms not involved in a reaction at a given timestep, and therefore should be used by a subsequent system-wide time integrator such as nvt, npt, or nve, as shown in the second example above (full examples can be found at examples/USER/misc/bond_react). The time integration command should be placed after the fix bond/react command due to the internal dynamic grouping performed by fix bond/react.

Note: If the group-ID is an existing static group, react-group-IDs should also be specified as this static group, or a subset.

The following comments pertain to each *react* argument (in other words, can be customized for each reaction, or reaction step):

A check for possible new reaction sites is performed every *Nevery* timesteps.

Three physical conditions must be met for a reaction to occur. First, a bonding atom pair must be identified within the reaction distance cutoffs. Second, the topology surrounding the bonding atom pair must match the topology of the pre-reaction template. Finally, any reaction constraints listed in the map file (see below) must be satisfied. If all of these conditions are met, the reaction site is eligible to be modified to match the post-reaction template.

A bonding atom pair will be identified if several conditions are met. First, a pair of atoms I,J within the specified react-group-ID of type itype and jtype must be separated by a distance between *Rmin* and *Rmax*. It is possible that multiple bonding atom pairs are identified: if the bonding atoms in the pre-reacted template are 1-2 neighbors, i.e. directly bonded, the farthest bonding atom partner is set as its bonding partner; otherwise, the closest potential partner is chosen. Then, if both an atom I and atom J have each other as their bonding partners, these two atoms are identified as the bonding atom pair of the reaction site. Once this unique bonding atom pair is identified for each reaction, there could two or more reactions that involve a given atom on the same timestep. If this is the case, only one such reaction is permitted to occur. This reaction is chosen randomly from all potential reactions. This capability allows e.g. for different reaction pathways to proceed from identical reaction sites with user-specified probabilities.

The pre-reacted molecule template is specified by a molecule command. This molecule template file contains a sample

reaction site and its surrounding topology. As described below, the bonding atom pairs of the pre-reacted template are specified by atom ID in the map file. The pre-reacted molecule template should contain as few atoms as possible while still completely describing the topology of all atoms affected by the reaction. For example, if the force field contains dihedrals, the pre-reacted template should contain any atom within three bonds of reacting atoms.

Some atoms in the pre-reacted template that are not reacting may have missing topology with respect to the simulation. For example, the pre-reacted template may contain an atom that, in the simulation, is currently connected to the rest of a long polymer chain. These are referred to as edge atoms, and are also specified in the map file. All pre-reaction template atoms should be linked to a bonding atom, via at least one path that does not involve edge atoms. When the pre-reaction template contains edge atoms, not all atoms, bonds, charges, etc. specified in the reaction templates will be updated. Specifically, topology that involves only atoms that are 'too near' to template edges will not be updated. The definition of 'too near the edge' depends on which interactions are defined in the simulation. If the simulation has defined dihedrals, atoms within two bonds of edge atoms are considered 'too near the edge.' If the simulation defines angles, but not dihedrals, atoms within one bond of edge atoms are considered 'too near the edge.' If just bonds are defined, only edge atoms are considered 'too near the edge.'

Note: Small molecules, i.e. ones that have all their atoms contained within the reaction templates, never have edge atoms.

Note that some care must be taken when a building a molecule template for a given simulation. All atom types in the pre-reacted template must be the same as those of a potential reaction site in the simulation. A detailed discussion of matching molecule template atom types with the simulation is provided on the *molecule* command page.

The post-reacted molecule template contains a sample of the reaction site and its surrounding topology after the reaction has occurred. It must contain the same number of atoms as the pre-reacted template. A one-to-one correspondence between the atom IDs in the pre- and post-reacted templates is specified in the map file as described below. Note that during a reaction, an atom, bond, etc. type may change to one that was previously not present in the simulation. These new types must also be defined during the setup of a given simulation. A discussion of correctly handling this is also provided on the *molecule* command page.

Note: When a reaction occurs, it is possible that the resulting topology/atom (e.g. special bonds, dihedrals, etc.) exceeds that of the existing system and reaction templates. As when inserting molecules, enough space for this increased topology/atom must be reserved by using the relevant "extra" keywords to the *read_data* or *create_box* commands.

The map file is a text document with the following format:

A map file has a header and a body. The header of map file the contains one mandatory keyword and five optional keywords. The mandatory keyword is 'equivalences':

```
N equivalences = # of atoms N in the reaction molecule templates
```

The optional keywords are 'edgeIDs', 'deleteIDs', 'customIDs' and 'constraints':

```
N edgeIDs = # of edge atoms N in the pre-reacted molecule template
N deleteIDs = # of atoms N that are specified for deletion
N chiralIDs = # of specified chiral centers N
N customIDs = # of atoms N that are specified for a custom update
N constraints = # of specified reaction constraints N
```

The body of the map file contains two mandatory sections and five optional sections. The first mandatory section begins with the keyword 'BondingIDs' and lists the atom IDs of the bonding atom pair in the pre-reacted molecule template. The second mandatory section begins with the keyword 'Equivalences' and lists a one-to-one correspondence between atom IDs of the pre- and post-reacted templates. The first column is an atom ID of the pre-reacted molecule template, and the second column is the corresponding atom ID of the post-reacted molecule template. The first optional section

begins with the keyword 'EdgeIDs' and lists the atom IDs of edge atoms in the pre-reacted molecule template. The second optional section begins with the keyword 'DeleteIDs' and lists the atom IDs of pre-reaction template atoms to delete. The third optional section begins with the keyword 'ChiralIDs' lists the atom IDs of chiral atoms whose handedness should be enforced. The fourth optional section begins with the keyword 'Custom Edges' and allows for forcing the update of a specific atom's atomic charge. The first column is the ID of an atom near the edge of the pre-reacted molecule template, and the value of the second column is either 'none' or 'charges.' Further details are provided in the discussion of the 'update_edges' keyword. The fifth optional section begins with the keyword 'Constraints' and lists additional criteria that must be satisfied in order for the reaction to occur. Currently, there are three types of constraints available, as discussed below.

A sample map file is given below:

```
# this is a map file

7 equivalences
2 edgeIDs

BondingIDs

3
5

EdgeIDs

1
7

Equivalences

1   1
2   2
3   3
4   4
5   5
6   6
7   7
```

The handedness of atoms that are chiral centers can be enforced by listing their IDs in the ChiralIDs section. A chiral atom must be bonded to four atoms with mutually different atom types. This feature uses the coordinates and types of the involved atoms in the pre-reaction template to determine handedness. Three atoms bonded to the chiral center are arbitrarily chosen, to define an oriented plane, and the relative position of the fourth bonded atom determines the chiral center's handedness.

Any number of additional constraints may be specified in the Constraints section of the map file. The constraint of type 'distance' has syntax as follows:

`distance` *`ID1 ID2 rmin rmax`*

where 'distance' is the required keyword, *ID1* and *ID2* are pre-reaction atom IDs, and these two atoms must be separated by a distance between *rmin* and *rmax* for the reaction to occur.

The constraint of type 'angle' has the following syntax:

`angle` *`ID1 ID2 ID3 amin amax`*

where 'angle' is the required keyword, *ID1*, *ID2* and *ID3* are pre-reaction atom IDs, and these three atoms must form an angle between *amin* and *amax* for the reaction to occur (where *ID2* is the central atom). Angles must be specified in degrees. This constraint can be used to enforce a certain orientation between reacting molecules.

The constraint of type 'arrhenius' imposes an additional reaction probability according to the temperature-dependent Arrhenius equation:

$$k = AT^n e^{\frac{-E_a}{k_B T}}$$

The Arrhenius constraint has the following syntax:

```
arrhenius A n E_a seed
```

where 'arrhenius' is the required keyword, *A* is the pre-exponential factor, *n* is the exponent of the temperature dependence, E_a is the activation energy (*units* of energy), and *seed* is a random number seed. The temperature is defined as the instantaneous temperature averaged over all atoms in the reaction site, and is calculated in the same manner as for example *compute temp/chunk*. Currently, there are no options for additional temperature averaging or velocity-biased temperature calculations. A uniform random number between 0 and 1 is generated using *seed*; if this number is less than the result of the Arrhenius equation above, the reaction is permitted to occur.

Once a reaction site has been successfully identified, data structures within LAMMPS that store bond topology are updated to reflect the post-reacted molecule template. All force fields with fixed bonds, angles, dihedrals or impropers are supported.

A few capabilities to note: 1) You may specify as many *react* arguments as desired. For example, you could break down a complicated reaction mechanism into several reaction steps, each defined by its own *react* argument. 2) While typically a bond is formed or removed between the bonding atom pairs specified in the pre-reacted molecule template, this is not required. 3) By reversing the order of the pre- and post- reacted molecule templates in another *react* argument, you can allow for the possibility of one or more reverse reactions.

The optional keywords deal with the probability of a given reaction occurring as well as the stable equilibration of each reaction site as it occurs:

The *prob* keyword can affect whether or not an eligible reaction actually occurs. The fraction setting must be a value between 0.0 and 1.0. A uniform random number between 0.0 and 1.0 is generated and the eligible reaction only occurs if the random number is less than the fraction. Up to N reactions are permitted to occur, as optionally specified by the *max_rxn* keyword.

The *stabilize_steps* keyword allows for the specification of how many timesteps a reaction site is stabilized before being returned to the overall system thermostat. In order to produce the most physical behavior, this 'reaction site equilibration time' should be tuned to be as small as possible while retaining stability for a given system or reaction step. After a limited number of case studies, this number has been set to a default of 60 timesteps. Ideally, it should be individually tuned for each fix reaction step. Note that in some situations, decreasing rather than increasing this parameter will result in an increase in stability.

The *update_edges* keyword can increase the number of atoms whose atomic charges are updated, when the pre-reaction template contains edge atoms. When the value is set to 'charges,' all atoms' atomic charges are updated to those specified by the post-reaction template, including atoms near the edge of reaction templates. When the value is set to 'custom,' an additional section must be included in the map file that specifies whether or not to update charges, on a per-atom basis. The format of this section is detailed above. Listing a pre-reaction atom ID with a value of 'charges' will force the update of the atom's charge, even if it is near a template edge. Atoms not near a template edge are unaffected by this setting.

A few other considerations:

Many reactions result in one or more atoms that are considered unwanted by-products. Therefore, bond/react provides the option to delete a user-specified set of atoms. These pre-reaction atoms are identified in the map file. A deleted atom must still be included in the post-reaction molecule template, in which it cannot be bonded to an atom that is not deleted. In addition to deleting unwanted reaction by-products, this feature can be used to remove specific topologies, such as small rings, that may be otherwise indistinguishable.

Optionally, you can enforce additional behaviors on reacting atoms. For example, it may be beneficial to force reacting atoms to remain at a certain temperature. For this, you can use the internally-created dynamic group named "bond_react_MASTER_group", which consists of all atoms currently involved in a reaction. For example, adding the following command would add an additional thermostat to the group of all currently-reacting atoms:

```
fix 1 bond_react_MASTER_group temp/rescale 1 300 300 10 1
```

Note: This command must be added after the fix bond/react command, and will apply to all reactions.

Computationally, each timestep this fix operates, it loops over neighbor lists (for bond-forming reactions) and computes distances between pairs of atoms in the list. It also communicates between neighboring processors to coordinate which bonds are created and/or removed. All of these operations increase the cost of a timestep. Thus you should be cautious about invoking this fix too frequently.

You can dump out snapshots of the current bond topology via the dump local command.

Restart, fix_modify, output, run start/stop, minimize info:

Cumulative reaction counts for each reaction are written to *binary restart files*. These values are associated with the reaction name (react-ID). Additionally, internally-created per-atom properties are stored to allow for smooth restarts. None of the *fix_modify* options are relevant to this fix.

This fix computes one statistic for each *react* argument that it stores in a global vector, of length 'number of react arguments', that can be accessed by various *output commands*. The vector values calculated by this fix are "intensive".

These is 1 quantity for each react argument:

- (1) cumulative # of reactions occurred

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

When fix bond/react is 'unfixed,' all internally-created groups are deleted. Therefore, fix bond/react can only be unfixed after unfixing all other fixes that use any group created by fix bond/react.

16.20.4 Restrictions

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.20.5 Related commands

fix bond/create, *fix bond/break*, *fix bond/swap*, *dump local*, *special_bonds*

16.20.6 Default

The option defaults are stabilization = no, prob = 1.0, stabilize_steps = 60, update_edges = none

---

(Gissinger) Gissinger, Jensen and Wise, Polymer, 128, 211 (2017).

16.21 fix bond/swap command

16.21.1 Syntax

```
fix ID group-ID bond/swap Nevery fraction cutoff seed
```

- ID, group-ID are documented in *fix* command
- bond/swap = style name of this fix command
- Nevery = attempt bond swapping every this many steps
- fraction = fraction of group atoms to consider for swapping
- cutoff = distance at which swapping will be considered (distance units)
- seed = random # seed (positive integer)

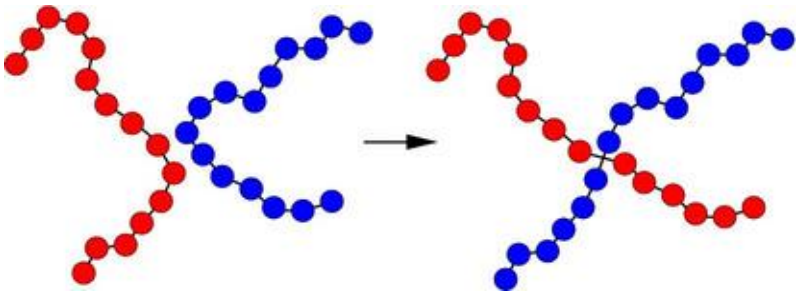
16.21.2 Examples

```
fix 1 all bond/swap 50 0.5 1.3 598934
```

16.21.3 Description

In a simulation of polymer chains, this command attempts to swap bonds between two different chains, effectively grafting the end of one chain onto another chain and vice versa. This is done via Monte Carlo rules using the Boltzmann acceptance criterion. The purpose is to equilibrate the polymer chain conformations more rapidly than dynamics alone would do it, by enabling instantaneous large conformational changes in a dense polymer melt. The polymer chains should thus more rapidly converge to the proper end-to-end distances and radii of gyration. It is designed for use with systems of *FENE* or *harmonic* bead-spring polymer chains where each polymer is a linear chain of monomers, but LAMMPS does not enforce this requirement, i.e. any *bond_style* can be used.

A schematic of the kinds of bond swaps that can occur is shown here:



On the left, the red and blue chains have two monomers A1 and B1 close to each other, which are currently bonded to monomers A2 and B2 respectively within their own chains. The bond swap operation will attempt to delete the

A1-A2 and B1-B2 bonds and replace them with A1-B2 and B1-A2 bonds. If the swap is energetically favorable, the two chains on the right are the result and each polymer chain has undergone a dramatic conformational change. This reference, *(Sides)* provides more details on how the algorithm works and its application:

The bond swapping operation is invoked every *Nevery* timesteps. If any bond is swapped, a re-build of the neighbor lists is triggered, since a swap alters the list of which neighbors are considered for pairwise interaction. At each invocation, each processor considers a random specified *fraction* of its atoms as potential swapping monomers for this timestep. Choosing a small *fraction* value can reduce the likelihood of a reverse swap occurring soon after an initial swap.

For each monomer A1, its neighbors are examined to find a possible B1 monomer. Both A1 and B1 must be in the fix group, their separation must be less than the specified *cutoff*, and the molecule IDs of A1 and B1 must be the same (see below). If a suitable partner is found, the energy change due to swapping the 2 bonds is computed. This includes changes in pairwise, bond, and angle energies due to the altered connectivity of the 2 chains. Dihedral and improper interactions are not allowed to be defined when this fix is used.

If the energy decreases due to the swap operation, the bond swap is accepted. If the energy increases it is accepted with probability exp(-delta/kT) where delta is the increase in energy, k is the Boltzmann constant, and T is the current temperature of the system. Whether the swap is accepted or rejected, no other swaps are attempted by this processor on this timestep.

The criterion for matching molecule IDs is how bond swaps performed by this fix conserve chain length. To use this features you must setup the molecule IDs for your polymer chains in a certain way, typically in the data file, read by the *read_data* command. Consider a system of 6-mer chains. You have 2 choices. If the molecule IDs for monomers on each chain are set to 1,2,3,4,5,6 then swaps will conserve chain length. For a particular monomer there will be only one other monomer on another chain which is a potential swap partner. If the molecule IDs for monomers on each chain are set to 1,2,3,3,2,1 then swaps will conserve chain length but swaps will be able to occur at either end of a chain. Thus for a particular monomer there will be 2 possible swap partners on another chain. In this scenario, swaps can also occur within a single chain, i.e. the two ends of a chain swap with each other.

Note: If your simulation uses molecule IDs in the usual way, where all monomers on a single chain are assigned the same ID (different for each chain), then swaps will only occur within the same chain. If you assign the same molecule ID to all monomers in all chains then inter-chain swaps will occur, but they will not conserve chain length. Neither of these scenarios is probably what you want for this fix.

Note: When a bond swap occurs the image flags of monomers in the new polymer chains can become inconsistent. See the *dump* command for a discussion of image flags. This is not an issue for running dynamics, but can affect calculation of some diagnostic quantities or the printing of unwrapped coordinates to a dump file.

This fix computes a temperature each time it is invoked for use by the Boltzmann criterion. To do this, the fix creates its own compute of style *temp*, as if this command had been issued:

```
compute fix-ID_temp all temp
```

See the *compute temp* command for details. Note that the ID of the new compute is the fix-ID with underscore + "temp" appended and the group for the new compute is "all", so that the temperature of the entire system is used.

Note that this is NOT the compute used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp*. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the *compute_modify* command or print this temperature during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* will have no effect on this fix.

Restart, fix_modify, thermo output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior. Also note that each processor generates possible swaps independently of other processors. Thus if you repeat the same simulation on a different number of processors, the specific swaps performed will be different.

The *fix_modify* *temp* option is supported by this fix. You can use it to assign a *compute* you have defined to this fix which will be used to compute the temperature for the Boltzmann criterion.

This fix computes two statistical quantities as a global 2-vector of output, which can be accessed by various *output commands*. The first component of the vector is the cumulative number of swaps performed by all processors. The second component of the vector is the cumulative number of swaps attempted (whether accepted or rejected). Note that a swap "attempt" only occurs when swap partners meeting the criteria described above are found on a particular timestep. The vector values calculated by this fix are "intensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.21.4 Restrictions

This fix is part of the MC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

The settings of the "special_bond" command must be 0,1,1 in order to use this fix, which is typical of bead-spring chains with FENE or harmonic bonds. This means that pairwise interactions between bonded atoms are turned off, but are turned on between atoms two or three hops away along the chain backbone.

Currently, energy changes in dihedral and improper interactions due to a bond swap are not considered. Thus a simulation that uses this fix cannot use a dihedral or improper potential.

16.21.5 Related commands

fix atom/swap

Default: none

(Sides) Sides, Grest, Stevens, Plimpton, J Polymer Science B, 42, 199-208 (2004).

16.22 fix box/relax command

16.22.1 Syntax

```
fix ID group-ID box/relax keyword value ...
```

- ID, group-ID are documented in *fix* command
- box/relax = style name of this fix command

```
one or more keyword value pairs may be appended
keyword = iso or aniso or tri or x or y or z or xy or yz or xz or␣
↪couple or nreset or vmax or dilate or scaleyz or scalexz or scalexy␣
↪or fixedpoint
```

```
  iso or aniso or tri value = Ptarget = desired pressure (pressure units)
  x or y or z or xy or yz or xz value = Ptarget = desired pressure␣
↪(pressure units)
  couple = none or xyz or xy or yz or xz
  nreset value = reset reference cell every this many minimizer iterations
  vmax value = fraction = max allowed volume change in one iteration
  dilate value = all or partial
  scaleyz value = yes or no = scale yz with lz
  scalexz value = yes or no = scale xz with lz
  scalexy value = yes or no = scale xy with ly
  fixedpoint values = x y z
    x,y,z = perform relaxation dilation/contraction around this point␣
↪(distance units)
```

16.22.2 Examples

```
fix 1 all box/relax iso 0.0 vmax 0.001
fix 2 water box/relax aniso 0.0 dilate partial
fix 2 ice box/relax tri 0.0 couple xy nreset 100
```

16.22.3 Description

Apply an external pressure or stress tensor to the simulation box during an *energy minimization*. This allows the box size and shape to vary during the iterations of the minimizer so that the final configuration will be both an energy minimum for the potential energy of the atoms, and the system pressure tensor will be close to the specified external tensor. Conceptually, specifying a positive pressure is like squeezing on the simulation box; a negative pressure typically allows the box to expand.

The external pressure tensor is specified using one or more of the *iso*, *aniso*, *tri*, *x*, *y*, *z*, *xy*, *xz*, *yz*, and *couple* keywords. These keywords give you the ability to specify all 6 components of an external stress tensor, and to couple various of these components together so that the dimensions they represent are varied together during the minimization.

Orthogonal simulation boxes have 3 adjustable dimensions (x,y,z). Triclinic (non-orthogonal) simulation boxes have 6 adjustable dimensions (x,y,z,xy,xz,yz). The *create_box*, *read data*, and *read_restart* commands specify whether the simulation box is orthogonal or non-orthogonal (triclinic) and explain the meaning of the xy,xz,yz tilt factors.

The target pressures *Ptarget* for each of the 6 components of the stress tensor can be specified independently via the *x*, *y*, *z*, *xy*, *xz*, *yz* keywords, which correspond to the 6 simulation box dimensions. For example, if the *y* keyword is used, the y-box length will change during the minimization. If the *xy* keyword is used, the xy tilt factor will change. A box dimension will not change if that component is not specified.

Note that in order to use the *xy*, *xz*, or *yz* keywords, the simulation box must be triclinic, even if its initial tilt factors are 0.0.

When the size of the simulation box changes, all atoms are re-scaled to new positions, unless the keyword *dilate* is specified with a value of *partial*, in which case only the atoms in the fix group are re-scaled. This can be useful for leaving the coordinates of atoms in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

The *scaleyz*, *scalexz*, and *scalexy* keywords control whether or not the corresponding tilt factors are scaled with the associated box dimensions when relaxing triclinic periodic cells. The default values *yes* will turn on scaling, which corresponds to adjusting the linear dimensions of the cell while preserving its shape. Choosing *no* ensures that the tilt factors are not scaled with the box dimensions. See below for restrictions and default values in different situations. In

older versions of LAMMPS, scaling of tilt factors was not performed. The old behavior can be recovered by setting all three scale keywords to *no*.

The *fixedpoint* keyword specifies the fixed point for cell relaxation. By default, it is the center of the box. Whatever point is chosen will not move during the simulation. For example, if the lower periodic boundaries pass through (0,0,0), and this point is provided to *fixedpoint*, then the lower periodic boundaries will remain at (0,0,0), while the upper periodic boundaries will move twice as far. In all cases, the particle positions at each iteration are unaffected by the chosen value, except that all particles are displaced by the same amount, different on each iteration.

Note: Applying an external pressure to tilt dimensions *xy*, *xz*, *yz* can sometimes result in arbitrarily large values of the tilt factors, i.e. a dramatically deformed simulation box. This typically indicates that there is something badly wrong with how the simulation was constructed. The two most common sources of this error are applying a shear stress to a liquid system or specifying an external shear stress tensor that exceeds the yield stress of the solid. In either case the minimization may converge to a bogus conformation or not converge at all. Also note that if the box shape tilts to an extreme shape, LAMMPS will run less efficiently, due to the large volume of communication needed to acquire ghost atoms around a processor's irregular-shaped sub-domain. For extreme values of tilt, LAMMPS may also lose atoms and generate an error.

Note: Performing a minimization with this fix is not a mathematically well-defined minimization problem. This is because the objective function being minimized changes if the box size/shape changes. In practice this means the minimizer can get "stuck" before you have reached the desired tolerance. The solution to this is to restart the minimizer from the new adjusted box size/shape, since that creates a new objective function valid for the new box size/shape. Repeat as necessary until the box size/shape has reached its new equilibrium.

The *couple* keyword allows two or three of the diagonal components of the pressure tensor to be "coupled" together. The value specified with the keyword determines which are coupled. For example, *xz* means the *Pxx* and *Pzz* components of the stress tensor are coupled. *Xyz* means all 3 diagonal components are coupled. Coupling means two things: the instantaneous stress will be computed as an average of the corresponding diagonal components, and the coupled box dimensions will be changed together in lockstep, meaning coupled dimensions will be dilated or contracted by the same percentage every timestep. The *Ptarget* values for any coupled dimensions must be identical. *Couple xyz* can be used for a 2d simulation; the *z* dimension is simply ignored.

The *iso*, *aniso*, and *tri* keywords are simply shortcuts that are equivalent to specifying several other keywords together.

The keyword *iso* means couple all 3 diagonal components together when pressure is computed (hydrostatic pressure), and dilate/contract the dimensions together. Using "iso Ptarget" is the same as specifying these 4 keywords:

```
x Ptarget
y Ptarget
z Ptarget
couple xyz
```

The keyword *aniso* means *x*, *y*, and *z* dimensions are controlled independently using the *Pxx*, *Pyy*, and *Pzz* components of the stress tensor as the driving forces, and the specified scalar external pressure. Using "aniso Ptarget" is the same as specifying these 4 keywords:

```
x Ptarget
y Ptarget
z Ptarget
couple none
```

The keyword *tri* means *x*, *y*, *z*, *xy*, *xz*, and *yz* dimensions are controlled independently using their individual stress components as the driving forces, and the specified scalar pressure as the external normal stress. Using "tri Ptarget" is the same as specifying these 7 keywords:

```
x Ptarget
y Ptarget
z Ptarget
xy 0.0
yz 0.0
xz 0.0
couple none
```

The *vmax* keyword can be used to limit the fractional change in the volume of the simulation box that can occur in one iteration of the minimizer. If the pressure is not settling down during the minimization this can be because the volume is fluctuating too much. The specified fraction must be greater than 0.0 and should be << 1.0. A value of 0.001 means the volume cannot change by more than 1/10 of a percent in one iteration when *couple xyz* has been specified. For any other case it means no linear dimension of the simulation box can change by more than 1/10 of a percent.

With this fix, the potential energy used by the minimizer is augmented by an additional energy provided by the fix. The overall objective function then is:

$$E = U + P_t \left(V - V_0\right) + E_{strain}$$

where U is the system potential energy, P_t is the desired hydrostatic pressure, V and V_0 are the system and reference volumes, respectively. E_{strain} is the strain energy expression proposed by Parrinello and Rahman *(Parrinello1981)*. Taking derivatives of E w.r.t. the box dimensions, and setting these to zero, we find that at the minimum of the objective function, the global system stress tensor $\mathbf{P}$ will satisfy the relation:

$$\mathbf{P} = P_t \mathbf{I} + \mathbf{S}_t \left(\mathbf{h}_0^{-1}\right)^t \mathbf{h}_{0d}$$

where $\mathbf{I}$ is the identity matrix, $\mathbf{h_0}$ is the box dimension tensor of the reference cell, and :$\mathbf{h_{0d}}$ is the diagonal part of $\mathbf{h_0}$. $\mathbf{S_t}$ is a symmetric stress tensor that is chosen by LAMMPS so that the upper-triangular components of $\mathbf{P}$ equal the stress tensor specified by the user.

This equation only applies when the box dimensions are equal to those of the reference dimensions. If this is not the case, then the converged stress tensor will not equal that specified by the user. We can resolve this problem by periodically resetting the reference dimensions. The keyword *nreset* controls how often this is done. If this keyword is not used, or is given a value of zero, then the reference dimensions are set to those of the initial simulation domain and are never changed. A value of *nstep* means that every *nstep* minimization steps, the reference dimensions are set to those of the current simulation domain. Note that resetting the reference dimensions changes the objective function and gradients, which sometimes causes the minimization to fail. This can be resolved by changing the value of *nreset*, or simply continuing the minimization from a restart file.

Note: As normally computed, pressure includes a kinetic- energy or temperature-dependent component; see the *compute pressure* command. However, atom velocities are ignored during a minimization, and the applied pressure(s) specified with this command are assumed to only be the virial component of the pressure (the non-kinetic portion). Thus if atoms have a non-zero temperature and you print the usual thermodynamic pressure, it may not appear the system is converging to your specified pressure. The solution for this is to either (a) zero the velocities of all atoms before performing the minimization, or (b) make sure you are monitoring the pressure without its kinetic component. The latter can be done by outputting the pressure from the pressure compute this command creates (see below) or a pressure compute you define yourself.

Note: Because pressure is often a very sensitive function of volume, it can be difficult for the minimizer to equilibrate the system the desired pressure with high precision, particularly for solids. Some techniques that seem to help are (a) use the "min_modify line quadratic" option when minimizing with box relaxations, (b) minimize several times in succession if need be, to drive the pressure closer to the target pressure, (c) relax the atom positions before relaxing the box, and (d) relax the box to the target hydrostatic pressure before relaxing to a target shear stress state. Also note that some systems (e.g. liquids) will not sustain a non-hydrostatic applied pressure, which means the minimizer will not converge.

This fix computes a temperature and pressure each timestep. The temperature is used to compute the kinetic contribution to the pressure, even though this is subsequently ignored by default. To do this, the fix creates its own computes of style "temp" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp group-ID temp
compute fix-ID_press group-ID pressure fix-ID_temp virial
```

See the *compute temp* and *compute pressure* commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is the same as the fix group. Also note that the pressure compute does not include a kinetic component.

Note that these are NOT the computes used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the *compute_modify* command or print this temperature or pressure during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify temp* and *press* options are supported by this fix. You can use them to assign a *compute* you have defined to this fix which will be used in its temperature and pressure calculation, as described above. Note that as described above, if you assign a pressure compute to this fix that includes a kinetic energy component it will affect the minimization, most likely in an undesirable way.

Note: If both the *temp* and *press* keywords are used in a single thermo_modify command (or in two separate commands), then the order in which the keywords are specified is important. Note that a *pressure compute* defines its own temperature compute as an argument when it is specified. The *temp* keyword will override this (for the pressure compute being used by fix box/relax), but only if the *temp* keyword comes after the *press* keyword. If the *temp* keyword comes before the *press* keyword, then the new pressure compute specified by the *press* keyword will be unaffected by the *temp* setting.

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the pressure-volume energy, plus the strain energy, if it exists, as described above. The energy values reported at the end of a minimization run under "Minimization stats" include this energy, and so differ from what LAMMPS normally reports as potential energy. This fix does not support the *fix_modify energy* option, because that would result in double-counting of the fix energy in the minimization energy. Instead, the fix energy can be explicitly added to the potential energy using one of these two variants:

```
variable emin equal pe+f_1

variable emin equal pe+f_1/atoms
```

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

This fix is invoked during *energy minimization*, but not for the purpose of adding a contribution to the energy or forces being minimized. Instead it alters the simulation box geometry as described above.

16.22.4 Restrictions

Only dimensions that are available can be adjusted by this fix. Non-periodic dimensions are not available. *z*, *xz*, and *yz*, are not available for 2D simulations. *xy*, *xz*, and *yz* are only available if the simulation domain is non-orthogonal. The *create_box*, *read data*, and *read_restart* commands specify whether the simulation box is orthogonal or non-orthogonal (triclinic) and explain the meaning of the xy,xz,yz tilt factors.

The *scaleyz yes* and *scalexz yes* keyword/value pairs can not be used for 2D simulations. *scaleyz yes*, *scalexz yes*, and *scalexy yes* options can only be used if the 2nd dimension in the keyword is periodic, and if the tilt factor is not coupled to the barostat via keywords *tri*, *yz*, *xz*, and *xy*.

16.22.5 Related commands

fix npt, *minimize*

16.22.6 Default

The keyword defaults are dilate = all, vmax = 0.0001, nreset = 0.

(Parrinello1981) Parrinello and Rahman, J Appl Phys, 52, 7182 (1981).

16.23 fix client/md command

16.23.1 Syntax

```
fix ID group-ID client/md
```

- ID, group-ID are documented in *fix* command
- client/md = style name of this fix command

16.23.2 Examples

```
fix 1 all client/md
```

16.23.3 Description

This fix style enables LAMMPS to run as a "client" code and communicate each timestep with a separate "server" code to perform an MD simulation together.

The *Howto client/server* doc page gives an overview of client/server coupling of LAMMPS with another code where one code is the "client" and sends request messages to a "server" code. The server responds to each request with a reply message. This enables the two codes to work in tandem to perform a simulation.

When using this fix, LAMMPS (as the client code) passes the current coordinates of all particles to the server code each timestep, which computes their interaction, and returns the energy, forces, and virial for the interacting particles to LAMMPS, so it can complete the timestep.

Note that the server code can be a quantum code, or another classical MD code which encodes a force field (pair_style in LAMMPS lingo) which LAMMPS does not have. In the quantum case, this fix is a mechanism for running *ab initio* MD with quantum forces.

The group associated with this fix is ignored.

The protocol and *units* for message format and content that LAMMPS exchanges with the server code is defined on the *server md* doc page.

Note that when using LAMMPS as an MD client, your LAMMPS input script should not normally contain force field commands, like a *pair_style*, *bond_style*, or *kspace_style* command. However it is possible for a server code to only compute a portion of the full force-field, while LAMMPS computes the remaining part. Your LAMMPS script can also specify boundary conditions or force constraints in the usual way, which will be added to the per-atom forces returned by the server code.

See the examples/message directory for example scripts where LAMMPS is both the "client" and/or "server" code for this kind of client/server MD simulation. The examples/message/README file explains how to launch LAMMPS and another code in tandem to perform a coupled simulation.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify* *energy* option is supported by this fix to add the potential energy computed by the server application to the system's potential energy as part of *thermodynamic output*.

The *fix_modify* *virial* option is supported by this fix to add the server application's contribution to the system's virial as part of *thermodynamic output*. The default is *virial yes*

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the potential energy discussed above. The scalar value calculated by this fix is "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.23.4 Restrictions

This fix is part of the MESSAGE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

A script that uses this command must also use the *message* command to setup and shut down the messaging protocol with the server code.

16.23.5 Related commands

message, *server*

Default: none

16.24 fix cmap command

16.24.1 Syntax

```
fix ID group-ID cmap filename
```

- ID, group-ID are documented in *fix* command
- cmap = style name of this fix command
- filename = force-field file with CMAP coefficients

16.24.2 Examples

```
fix             myCMAP all cmap ../potentials/cmap36.data
read_data       proteinX.data fix myCMAP crossterm CMAP
fix_modify      myCMAP energy yes
```

16.24.3 Description

This command enables CMAP cross-terms to be added to simulations which use the CHARMM force field. These are relevant for any CHARMM model of a peptide or protein sequences that is 3 or more amino-acid residues long; see *(Buck)* and *(Brooks)* for details, including the analytic energy expressions for CMAP interactions. The CMAP cross-terms add additional potential energy contributions to pairs of overlapping phi-psi dihedrals of amino-acids, which are important to properly represent their conformational behavior.

The examples/cmap directory has a sample input script and data file for a small peptide, that illustrates use of the fix cmap command.

As in the example above, this fix should be used before reading a data file that contains a listing of CMAP interactions. The *filename* specified should contain the CMAP parameters for a particular version of the CHARMM force field. Two such files are including in the lammps/potentials directory: charmm22.cmap and charmm36.cmap.

The data file read by the "read_data" must contain the topology of all the CMAP interactions, similar to the topology data for bonds, angles, dihedrals, etc. Specially it should have a line like this in its header section:

```
N crossterms
```

where N is the number of CMAP cross-terms. It should also have a section in the body of the data file like this with N lines:

```
CMAP

       1       1       8      10      12      18      20
       2       5      18      20      22      25      27
       [...]
       N       3     314     315     317     318     330
```

The first column is an index from 1 to N to enumerate the CMAP terms; it is ignored by LAMMPS. The 2nd column is the "type" of the interaction; it is an index into the CMAP force field file. The remaining 5 columns are the atom IDs of the atoms in the two 4-atom dihedrals that overlap to create the CMAP 5-body interaction. Note that the "crossterm" and "CMAP" keywords for the header and body sections match those specified in the read_data command following the data file name; see the *read_data* doc page for more details.

A data file containing CMAP cross-terms can be generated from a PDB file using the charmm2lammps.pl script in the tools/ch2lmp directory of the LAMMPS distribution. The script must be invoked with the optional "-cmap" flag to do this; see the tools/ch2lmp/README file for more information.

The potential energy associated with CMAP interactions can be output as described below. It can also be included in the total potential energy of the system, as output by the *thermo_style* command, if the *fix_modify energy* command is used, as in the example above. See the note below about how to include the CMAP energy when performing an *energy minimization*.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the list of CMAP cross-terms to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify energy* option is supported by this fix to add the potential "energy" of the CMAP interactions system's potential energy as part of *thermodynamic output*.

The *fix_modify virial* option is supported by this fix to add the contribution due to the interaction between atoms to the system's virial as part of *thermodynamic output*. The default is *virial yes*

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the potential energy discussed above. The scalar value calculated by this fix is "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command.

Note: If you want the potential energy associated with the CMAP terms forces to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the *fix_modify energy* option for this fix.

16.24.4 Restrictions

To function as expected this fix command must be issued *before* a *read_data* command but *after* a *read_restart* command.

This fix can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

16.24.5 Related commands

fix_modify, *read_data*

Default: none

(Buck) Buck, Bouguet-Bonnet, Pastor, MacKerell Jr., Biophys J, 90, L36 (2006).

(Brooks) Brooks, Brooks, MacKerell Jr., J Comput Chem, 30, 1545 (2009).

16.25 fix colvars command

16.25.1 Syntax

```
fix ID group-ID colvars configfile keyword values ...
```

- ID, group-ID are documented in *fix* command
- colvars = style name of this fix command
- configfile = the configuration file for the colvars module
- keyword = *input* or *output* or *seed* or *tstat*

```
input arg = colvars.state file name or prefix or NULL (default: NULL)
output arg = output filename prefix (default: out)
seed arg = seed for random number generator (default: 1966)
unwrap arg = yes or no
  use unwrapped coordinates in collective variables (default: yes)
tstat arg = fix id of a thermostat or NULL (default: NULL)
```

16.25.2 Examples

```
fix mtd all colvars peptide.colvars.inp seed 2122 input peptide.colvars.state output␣
↪peptide
fix abf all colvars colvars.inp tstat 1
```

16.25.3 Description

This fix interfaces LAMMPS to the collective variables "Colvars" library, which allows to calculate potentials of mean force (PMFs) for any set of colvars, using different sampling methods: currently implemented are the Adaptive Biasing Force (ABF) method, metadynamics, Steered Molecular Dynamics (SMD) and Umbrella Sampling (US) via a flexible harmonic restraint bias.

This documentation describes only the fix colvars command itself and LAMMPS specific parts of the code. The full documentation of the colvars library is available as this supplementary PDF document

The Colvars library is developed at https://github.com/colvars/colvars A detailed discussion of its implementation is in *(Fiorin)*.

There are some example scripts for using this package with LAMMPS in the examples/USER/colvars directory.

The only mandatory argument to the fix is the filename to the colvars input file that contains the input that is independent from the MD program in which the colvars library has been integrated.

The *group-ID* entry is ignored. The collective variable module will always apply to the entire system and there can only be one instance of the colvars fix at a time. The colvars fix will only communicate the minimum information necessary and the colvars library supports multiple, completely independent collective variables, so there is no restriction to functionality by limiting the number of colvars fixes.

The *input* keyword allows to specify a state file that would contain the restart information required in order to continue a calculation from a prerecorded state. Fix colvars records it state in *binary restart* files, so when using the *read_restart* command, this is usually not needed.

The *output* keyword allows to specify the output prefix. All output files generated will use this prefix followed by the ".colvars." and a word like "state" or "traj".

The *seed* keyword contains the seed for the random number generator that will be used in the colvars module.

The *unwrap* keyword controls whether wrapped or unwrapped coordinates are passed to the colvars library for calculation of the collective variables and the resulting forces. The default is *yes*, i.e. to use the image flags to reconstruct the absolute atom positions. Setting this to *no* will use the current local coordinates that are wrapped back into the simulation cell at each re-neighboring instead.

The *tstat* keyword can be either NULL or the label of a thermostatting fix that thermostats all atoms in the fix colvars group. This will be used to provide the colvars module with the current thermostat target temperature.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the current status of the colvars module into *binary restart files*. This is in addition to the text mode status file that is written by the colvars module itself and the kind of information in both files is identical.

The *fix_modify energy* option is supported by this fix to add the energy change from the biasing force added by the fix to the system's potential energy as part of *thermodynamic output*.

The *fix_modify configfile* <*config file*> option allows to add settings from an additional config file to the colvars module. This option can only be used, after the system has been initialized with a *run* command.

The *fix_modify config* <*quoted string*> option allows to add settings from inline strings. Those have to fit on a single line when enclosed in a pair of double quotes ("), or can span multiple lines when bracketed by a pair of triple double quotes (""", like python embedded documentation).

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the cumulative energy change due to this fix. The scalar value calculated by this fix is "extensive".

16.25.4 Restrictions

This fix is part of the USER-COLVARS package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

There can only be one colvars fix active at a time. Since the interface communicates only the minimum amount of information and colvars module itself can handle an arbitrary number of collective variables, this is not a limitation of functionality.

16.25.5 Related commands

fix smd, *fix spring*, *fix plumed*

16.25.6 Default

The default options are input = NULL, output = out, seed = 1966, unwrap yes, and tstat = NULL.

(Fiorin) Fiorin, Klein, Henin, Mol. Phys., DOI:10.1080/00268976.2013.813594

16.26 fix controller command

16.26.1 Syntax

```
fix ID group-ID controller Nevery alpha Kp Ki Kd pvar setpoint cvar
```

- ID, group-ID are documented in *fix* command
- controller = style name of this fix command
- Nevery = invoke controller every this many timesteps
- alpha = coupling constant for PID equation (see units discussion below)
- Kp = proportional gain in PID equation (unitless)
- Ki = integral gain in PID equation (unitless)
- Kd = derivative gain in PID equation (unitless)
- pvar = process variable of form c_ID, c_ID[I], f_ID, f_ID[I], or v_name

```
c_ID = global scalar calculated by a compute with ID
c_ID[I] = Ith component of global vector calculated by a compute with ID
f_ID = global scalar calculated by a fix with ID
f_ID[I] = Ith component of global vector calculated by a fix with ID
v_name = value calculated by an equal-style variable with name
```

- setpoint = desired value of process variable (same units as process variable)
- cvar = name of control variable

16.26.2 Examples

```
fix 1 all controller 100 1.0 0.5 0.0 0.0 c_thermo_temp 1.5 tcontrol
fix 1 all controller 100 0.2 0.5 0 100.0 v_pxxwall 1.01325 xwall
fix 1 all controller 10000 0.2 0.5 0 2000 v_avpe -3.785 tcontrol
```

16.26.3 Description

This fix enables control of a LAMMPS simulation using a control loop feedback mechanism known as a proportional-integral-derivative (PID) controller. The basic idea is to define a "process variable" which is a quantity that can be monitored during a running simulation. A desired target value is chosen for the process variable. A "control variable" is also defined which is an adjustable attribute of the running simulation, which the process variable will respond to. The PID controller continuously adjusts the control variable based on the difference between the process variable and the target.

Here are examples of ways in which this fix can be used. The examples/pid directory contains a script that implements the simple thermostat.

Goal	process variable	control variable
Simple thermostat	instantaneous T	thermostat target T
Find melting temperature	average PE per atom	thermostat target T
Control pressure in non-periodic system	force on wall	position of wall

Note: For this fix to work, the control variable must actually induce a change in a running LAMMPS simulation. Typically this will only occur if there is some other command (e.g. a thermostat fix) which uses the control variable as an input parameter. This could be done directly or indirectly, e.g. the other command uses a variable as input whose formula uses the control variable. The other command should alter its behavior dynamically as the variable changes.

Note: If there is a command you think could be used in this fashion, but does not currently allow a variable as an input parameter, please notify the LAMMPS developers. It is often not difficult to enable a command to use a variable as an input parameter.

The group specified with this command is ignored. However, note that the process variable may be defined by calculations performed by computes and fixes which store their own "group" definitions.

The PID controller is invoked once each *Nevery* timesteps.

The PID controller is implemented as a discretized version of the following dynamic equation:

$$\frac{dc}{dt} = \hat{E} - \alpha(K_p e + K_i \int_0^t e\,dt + K_d \frac{de}{dt})$$

where *c* is the continuous time analog of the control variable, *e =pvar-setpoint* is the error in the process variable, and α, K_p, K_i , and K_d are constants set by the corresponding keywords described above. The discretized version of this equation is:

$$c_n = \hat{E} c_{n-1} - \alpha \left(K_p \tau e_n + K_i \tau^2 \sum_{i=1}^{n} e_i + K_d (e_n - e_{n-1}) \right)$$

where $\tau = \texttt{Nevery} \cdot \texttt{timestep}$ is the time interval between updates, and the subscripted variables indicate the values of *c* and *e* at successive updates.

From the first equation, it is clear that if the three gain values K_p, K_i, K_d are dimensionless constants, then α must have units of [unit *cvar*]/[unit *pvar*]/[unit time] e.g. [eV/K/ps]. The advantage of this unit scheme is that the value of the constants should be invariant under a change of either the MD timestep size or the value of *Nevery*. Similarly, if the LAMMPS *unit style* is changed, it should only be necessary to change the value of α to reflect this, while leaving K_p, K_i, and K_d unaltered.

When choosing the values of the four constants, it is best to first pick a value and sign for α that is consistent with the magnitudes and signs of *pvar* and *cvar*. The magnitude of K_p should then be tested over a large positive range keeping $K_i = K_d = 0$. A good value for K_p will produce a fast response in *pvar*, without overshooting the *setpoint*. For many applications, proportional feedback is sufficient, and so K_i = K_d =0` can be used. In cases where there is a substantial lag time in the response of *pvar* to a change in *cvar*, this can be counteracted by increasing K_d. In situations where *pvar* plateaus without reaching *setpoint*, this can be counteracted by increasing K_i. In the language of Charles Dickens, K_p represents the error of the present, K_i the error of the past, and K_d the error yet to come.

Because this fix updates *cvar*, but does not initialize its value, the initial value is that assigned by the user in the input script via the *internal-style variable* command. This value is used (by the other LAMMPS command that used the variable) until this fix performs its first update of *cvar* after *Nevery* timesteps. On the first update, the value of the derivative term is set to zero, because the value of $e_n - 1$ is not yet defined.

The process variable *pvar* can be specified as the output of a *compute* or *fix* or the evaluation of a *variable*. In each case, the compute, fix, or variable must produce a global quantity, not a per-atom or local quantity.

If *pvar* begins with "c_", a compute ID must follow which has been previously defined in the input script and which generates a global scalar or vector. See the individual *compute* doc page for details. If no bracketed integer is appended,

the scalar calculated by the compute is used. If a bracketed integer is appended, the Ith value of the vector calculated by the compute is used. Users can also write code for their own compute styles and *add them to LAMMPS*.

If *pvar* begins with "f_", a fix ID must follow which has been previously defined in the input script and which generates a global scalar or vector. See the individual *fix* doc page for details. Note that some fixes only produce their values on certain timesteps, which must be compatible with when fix controller references the values, or else an error results. If no bracketed integer is appended, the scalar calculated by the fix is used. If a bracketed integer is appended, the Ith value of the vector calculated by the fix is used. Users can also write code for their own fix style and *add them to LAMMPS*.

If *pvar* begins with "v_", a variable name must follow which has been previously defined in the input script. Only equal-style variables can be referenced. See the *variable* command for details. Note that variables of style *equal* define a formula which can reference individual atom properties or thermodynamic keywords, or they can invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of specifying the process variable.

The target value *setpoint* for the process variable must be a numeric value, in whatever units *pvar* is defined for.

The control variable *cvar* must be the name of an *internal-style variable* previously defined in the input script. Note that it is not specified with a "v_" prefix, just the name of the variable. It must be an internal-style variable, because this fix updates its value directly. Note that other commands can use an equal-style versus internal-style variable interchangeably.

Restart, fix_modify, output, run start/stop, minimize info:

Currently, no information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix produces a global vector with 3 values which can be accessed by various *output commands*. The values can be accessed on any timestep, though they are only updated on timesteps that are a multiple of *Nevery*.

The three values are the most recent updates made to the control variable by each of the 3 terms in the PID equation above. The first value is the proportional term, the second is the integral term, the third is the derivative term.

The units of the vector values will be whatever units the control variable is in. The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.26.4 Restrictions

none

16.26.5 Related commands

fix adapt

Default: none

16.27 fix deform command

16.28 fix deform/kk command

16.28.1 Syntax

```
fix ID group-ID deform N parameter args ... keyword value ...
```

- ID, group-ID are documented in *fix* command
- deform = style name of this fix command
- N = perform box deformation every this many timesteps
- one or more parameter/arg pairs may be appended

```
parameter = x or y or z or xy or xz or yz
  x, y, z args = style value(s)
    style = final or delta or scale or vel or erate or trate or volume or␣
↪wiggle or variable
      final values = lo hi
        lo hi = box boundaries at end of run (distance units)
      delta values = dlo dhi
        dlo dhi = change in box boundaries at end of run (distance units)
      scale values = factor
        factor = multiplicative factor for change in box length at end of␣
↪run
      vel value = V
        V = change box length at this velocity (distance/time units),
            effectively an engineering strain rate
      erate value = R
        R = engineering strain rate (1/time units)
      trate value = R
        R = true strain rate (1/time units)
      volume value = none = adjust this dim to preserve volume of system
      wiggle values = A Tp
        A = amplitude of oscillation (distance units)
        Tp = period of oscillation (time units)
      variable values = v_name1 v_name2
        v_name1 = variable with name1 for box length change as function␣
↪of time
        v_name2 = variable with name2 for change rate as function of time
  xy, xz, yz args = style value
    style = final or delta or vel or erate or trate or wiggle
      final value = tilt
        tilt = tilt factor at end of run (distance units)
      delta value = dtilt
        dtilt = change in tilt factor at end of run (distance units)
      vel value = V
        V = change tilt factor at this velocity (distance/time units),
            effectively an engineering shear strain rate
      erate value = R
        R = engineering shear strain rate (1/time units)
      trate value = R
```

```
      R = true shear strain rate (1/time units)
    wiggle values = A Tp
      A = amplitude of oscillation (distance units)
      Tp = period of oscillation (time units)
    variable values = v_name1 v_name2
      v_name1 = variable with name1 for tilt change as function of time
      v_name2 = variable with name2 for change rate as function of time
```

- zero or more keyword/value pairs may be appended
- keyword = *remap* or *flip* or *units*

```
remap value = x or v or none
  x = remap coords of atoms in group into deforming box
  v = remap velocities of all atoms when they cross periodic boundaries
  none = no remapping of x or v
flip value = yes or no
  allow or disallow box flips when it becomes highly skewed
units value = lattice or box
  lattice = distances are defined in lattice units
  box = distances are defined in simulation box units
```

16.28.2 Examples

```
fix 1 all deform 1 x final 0.0 9.0 z final 0.0 5.0 units box
fix 1 all deform 1 x trate 0.1 y volume z volume
fix 1 all deform 1 xy erate 0.001 remap v
fix 1 all deform 10 y delta -0.5 0.5 xz vel 1.0
```

16.28.3 Description

Change the volume and/or shape of the simulation box during a dynamics run. Orthogonal simulation boxes have 3 adjustable parameters (x,y,z). Triclinic (non-orthogonal) simulation boxes have 6 adjustable parameters (x,y,z,xy,xz,yz). Any or all of them can be adjusted independently and simultaneously by this command.

This fix can be used to perform non-equilibrium MD (NEMD) simulations of a continuously strained system. See the *fix nvt/sllod* and *compute temp/deform* commands for more details. Note that simulation of a continuously extended system (extensional flow) can be modeled using the *USER-UEF package* and its *fix commands*.

For the *x*, *y*, *z* parameters, the associated dimension cannot be shrink-wrapped. For the *xy*, *yz*, *xz* parameters, the associated 2nd dimension cannot be shrink-wrapped. Dimensions not varied by this command can be periodic or non-periodic. Dimensions corresponding to unspecified parameters can also be controlled by a *fix npt* or *fix nph* command.

The size and shape of the simulation box at the beginning of the simulation run were either specified by the *create_box* or *read_data* or *read_restart* command used to setup the simulation initially if it is the first run, or they are the values from the end of the previous run. The *create_box*, *read data*, and *read_restart* commands specify whether the simulation box is orthogonal or non-orthogonal (triclinic) and explain the meaning of the xy,xz,yz tilt factors. If fix deform changes the xy,xz,yz tilt factors, then the simulation box must be triclinic, even if its initial tilt factors are 0.0.

As described below, the desired simulation box size and shape at the end of the run are determined by the parameters of the fix deform command. Every Nth timestep during the run, the simulation box is expanded, contracted, or tilted to ramped values between the initial and final values.

For the *x*, *y*, and *z* parameters, this is the meaning of their styles and values.

The *final*, *delta*, *scale*, *vel*, and *erate* styles all change the specified dimension of the box via "constant displacement" which is effectively a "constant engineering strain rate". This means the box dimension changes linearly with time from its initial to final value.

For style *final*, the final lo and hi box boundaries of a dimension are specified. The values can be in lattice or box distance units. See the discussion of the units keyword below.

For style *delta*, plus or minus changes in the lo/hi box boundaries of a dimension are specified. The values can be in lattice or box distance units. See the discussion of the units keyword below.

For style *scale*, a multiplicative factor to apply to the box length of a dimension is specified. For example, if the initial box length is 10, and the factor is 1.1, then the final box length will be 11. A factor less than 1.0 means compression.

For style *vel*, a velocity at which the box length changes is specified in units of distance/time. This is effectively a "constant engineering strain rate", where rate = V/L0 and L0 is the initial box length. The distance can be in lattice or box distance units. See the discussion of the units keyword below. For example, if the initial box length is 100 Angstroms, and V is 10 Angstroms/psec, then after 10 psec, the box length will have doubled. After 20 psec, it will have tripled.

The *erate* style changes a dimension of the box at a "constant engineering strain rate". The units of the specified strain rate are 1/time. See the *units* command for the time units associated with different choices of simulation units, e.g. picoseconds for "metal" units). Tensile strain is unitless and is defined as delta/L0, where L0 is the original box length and delta is the change relative to the original length. The box length L as a function of time will change as

```
L(t) = L0 (1 + erate*dt)
```

where dt is the elapsed time (in time units). Thus if *erate* R is specified as 0.1 and time units are picoseconds, this means the box length will increase by 10% of its original length every picosecond. I.e. strain after 1 psec = 0.1, strain after 2 psec = 0.2, etc. R = -0.01 means the box length will shrink by 1% of its original length every picosecond. Note that for an "engineering" rate the change is based on the original box length, so running with R = 1 for 10 picoseconds expands the box length by a factor of 11 (strain of 10), which is different that what the *trate* style would induce.

The *trate* style changes a dimension of the box at a "constant true strain rate". Note that this is not an "engineering strain rate", as the other styles are. Rather, for a "true" rate, the rate of change is constant, which means the box dimension changes non-linearly with time from its initial to final value. The units of the specified strain rate are 1/time. See the *units* command for the time units associated with different choices of simulation units, e.g. picoseconds for "metal" units). Tensile strain is unitless and is defined as delta/L0, where L0 is the original box length and delta is the change relative to the original length.

The box length L as a function of time will change as

```
L(t) = L0 exp(trate*dt)
```

where dt is the elapsed time (in time units). Thus if *trate* R is specified as ln(1.1) and time units are picoseconds, this means the box length will increase by 10% of its current (not original) length every picosecond. I.e. strain after 1 psec = 0.1, strain after 2 psec = 0.21, etc. R = ln(2) or ln(3) means the box length will double or triple every picosecond. R = ln(0.99) means the box length will shrink by 1% of its current length every picosecond. Note that for a "true" rate the change is continuous and based on the current length, so running with R = ln(2) for 10 picoseconds does not expand the box length by a factor of 11 as it would with *erate*, but by a factor of 1024 since the box length will double every picosecond.

Note that to change the volume (or cross-sectional area) of the simulation box at a constant rate, you can change multiple dimensions via *erate* or *trate*. E.g. to double the box volume in a picosecond picosecond, you could set "x erate M", "y erate M", "z erate M", with M = pow(2,1/3) - 1 = 0.26, since if each box dimension grows by 26%, the box volume doubles. Or you could set "x trate M", "y trate M", "z trate M", with M = ln(1.26) = 0.231, and the box volume would double every picosecond.

The *volume* style changes the specified dimension in such a way that the box volume remains constant while other box dimensions are changed explicitly via the styles discussed above. For example, "x scale 1.1 y scale 1.1 z volume" will shrink the z box length as the x,y box lengths increase, to keep the volume constant (product of x,y,z lengths). If "x

scale 1.1 z volume" is specified and parameter *y* is unspecified, then the z box length will shrink as x increases to keep the product of x,z lengths constant. If "x scale 1.1 y volume z volume" is specified, then both the y,z box lengths will shrink as x increases to keep the volume constant (product of x,y,z lengths). In this case, the y,z box lengths shrink so as to keep their relative aspect ratio constant.

For solids or liquids, note that when one dimension of the box is expanded via fix deform (i.e. tensile strain), it may be physically undesirable to hold the other 2 box lengths constant (unspecified by fix deform) since that implies a density change. Using the *volume* style for those 2 dimensions to keep the box volume constant may make more physical sense, but may also not be correct for materials and potentials whose Poisson ratio is not 0.5. An alternative is to use *fix npt aniso* with zero applied pressure on those 2 dimensions, so that they respond to the tensile strain dynamically.

The *wiggle* style oscillates the specified box length dimension sinusoidally with the specified amplitude and period. I.e. the box length L as a function of time is given by

```
L(t) = L0 + A sin(2*pi t/Tp)
```

where L0 is its initial length. If the amplitude A is a positive number the box initially expands, then contracts, etc. If A is negative then the box initially contracts, then expands, etc. The amplitude can be in lattice or box distance units. See the discussion of the units keyword below.

The *variable* style changes the specified box length dimension by evaluating a variable, which presumably is a function of time. The variable with *name1* must be an *equal-style variable* and should calculate a change in box length in units of distance. Note that this distance is in box units, not lattice units; see the discussion of the *units* keyword below. The formula associated with variable *name1* can reference the current timestep. Note that it should return the "change" in box length, not the absolute box length. This means it should evaluate to 0.0 when invoked on the initial timestep of the run following the definition of fix deform. It should evaluate to a value > 0.0 to dilate the box at future times, or a value < 0.0 to compress the box.

The variable *name2* must also be an *equal-style variable* and should calculate the rate of box length change, in units of distance/time, i.e. the time-derivative of the *name1* variable. This quantity is used internally by LAMMPS to reset atom velocities when they cross periodic boundaries. It is computed internally for the other styles, but you must provide it when using an arbitrary variable.

Here is an example of using the *variable* style to perform the same box deformation as the *wiggle* style formula listed above, where we assume that the current timestep = 0.

```
variable A equal 5.0
variable Tp equal 10.0
variable displace equal "v_A * sin(2*PI * step*dt/v_Tp)"
variable rate equal "2*PI*v_A/v_Tp * cos(2*PI * step*dt/v_Tp)"
fix 2 all deform 1 x variable v_displace v_rate remap v
```

For the *scale*, *vel*, *erate*, *trate*, *volume*, *wiggle*, and *variable* styles, the box length is expanded or compressed around its mid point.

For the *xy*, *xz*, and *yz* parameters, this is the meaning of their styles and values. Note that changing the tilt factors of a triclinic box does not change its volume.

The *final*, *delta*, *vel*, and *erate* styles all change the shear strain at a "constant engineering shear strain rate". This means the tilt factor changes linearly with time from its initial to final value.

For style *final*, the final tilt factor is specified. The value can be in lattice or box distance units. See the discussion of the units keyword below.

For style *delta*, a plus or minus change in the tilt factor is specified. The value can be in lattice or box distance units. See the discussion of the units keyword below.

For style *vel*, a velocity at which the tilt factor changes is specified in units of distance/time. This is effectively an "engineering shear strain rate", where rate = V/L0 and L0 is the initial box length perpendicular to the direction

of shear. The distance can be in lattice or box distance units. See the discussion of the units keyword below. For example, if the initial tilt factor is 5 Angstroms, and the V is 10 Angstroms/psec, then after 1 psec, the tilt factor will be 15 Angstroms. After 2 psec, it will be 25 Angstroms.

The *erate* style changes a tilt factor at a "constant engineering shear strain rate". The units of the specified shear strain rate are 1/time. See the *units* command for the time units associated with different choices of simulation units, e.g. picoseconds for "metal" units). Shear strain is unitless and is defined as offset/length, where length is the box length perpendicular to the shear direction (e.g. y box length for xy deformation) and offset is the displacement distance in the shear direction (e.g. x direction for xy deformation) from the unstrained orientation.

The tilt factor T as a function of time will change as

```
T(t) = T0 + L0*erate*dt
```

where T0 is the initial tilt factor, L0 is the original length of the box perpendicular to the shear direction (e.g. y box length for xy deformation), and dt is the elapsed time (in time units). Thus if *erate* R is specified as 0.1 and time units are picoseconds, this means the shear strain will increase by 0.1 every picosecond. I.e. if the xy shear strain was initially 0.0, then strain after 1 psec = 0.1, strain after 2 psec = 0.2, etc. Thus the tilt factor would be 0.0 at time 0, 0.1*ybox at 1 psec, 0.2*ybox at 2 psec, etc, where ybox is the original y box length. R = 1 or 2 means the tilt factor will increase by 1 or 2 every picosecond. R = -0.01 means a decrease in shear strain by 0.01 every picosecond.

The *trate* style changes a tilt factor at a "constant true shear strain rate". Note that this is not an "engineering shear strain rate", as the other styles are. Rather, for a "true" rate, the rate of change is constant, which means the tilt factor changes non-linearly with time from its initial to final value. The units of the specified shear strain rate are 1/time. See the *units* command for the time units associated with different choices of simulation units, e.g. picoseconds for "metal" units). Shear strain is unitless and is defined as offset/length, where length is the box length perpendicular to the shear direction (e.g. y box length for xy deformation) and offset is the displacement distance in the shear direction (e.g. x direction for xy deformation) from the unstrained orientation.

The tilt factor T as a function of time will change as

```
T(t) = T0 exp(trate*dt)
```

where T0 is the initial tilt factor and dt is the elapsed time (in time units). Thus if *trate* R is specified as ln(1.1) and time units are picoseconds, this means the shear strain or tilt factor will increase by 10% every picosecond. I.e. if the xy shear strain was initially 0.1, then strain after 1 psec = 0.11, strain after 2 psec = 0.121, etc. R = ln(2) or ln(3) means the tilt factor will double or triple every picosecond. R = ln(0.99) means the tilt factor will shrink by 1% every picosecond. Note that the change is continuous, so running with R = ln(2) for 10 picoseconds does not change the tilt factor by a factor of 10, but by a factor of 1024 since it doubles every picosecond. Note that the initial tilt factor must be non-zero to use the *trate* option.

Note that shear strain is defined as the tilt factor divided by the perpendicular box length. The *erate* and *trate* styles control the tilt factor, but assume the perpendicular box length remains constant. If this is not the case (e.g. it changes due to another fix deform parameter), then this effect on the shear strain is ignored.

The *wiggle* style oscillates the specified tilt factor sinusoidally with the specified amplitude and period. I.e. the tilt factor T as a function of time is given by

```
T(t) = T0 + A sin(2*pi t/Tp)
```

where T0 is its initial value. If the amplitude A is a positive number the tilt factor initially becomes more positive, then more negative, etc. If A is negative then the tilt factor initially becomes more negative, then more positive, etc. The amplitude can be in lattice or box distance units. See the discussion of the units keyword below.

The *variable* style changes the specified tilt factor by evaluating a variable, which presumably is a function of time. The variable with *name1* must be an *equal-style variable* and should calculate a change in tilt in units of distance. Note that this distance is in box units, not lattice units; see the discussion of the *units* keyword below. The formula associated with variable *name1* can reference the current timestep. Note that it should return the "change" in tilt factor, not the absolute tilt factor. This means it should evaluate to 0.0 when invoked on the initial timestep of the run following the definition of fix deform.

The variable *name2* must also be an *equal-style variable* and should calculate the rate of tilt change, in units of distance/time, i.e. the time-derivative of the *name1* variable. This quantity is used internally by LAMMPS to reset atom velocities when they cross periodic boundaries. It is computed internally for the other styles, but you must provide it when using an arbitrary variable.

Here is an example of using the *variable* style to perform the same box deformation as the *wiggle* style formula listed above, where we assume that the current timestep = 0.

```
variable A equal 5.0
variable Tp equal 10.0
variable displace equal "v_A * sin(2*PI * step*dt/v_Tp)"
variable rate equal "2*PI*v_A/v_Tp * cos(2*PI * step*dt/v_Tp)"
fix 2 all deform 1 xy variable v_displace v_rate remap v
```

All of the tilt styles change the xy, xz, yz tilt factors during a simulation. In LAMMPS, tilt factors (xy,xz,yz) for triclinic boxes are normally bounded by half the distance of the parallel box length. See the discussion of the *flip* keyword below, to allow this bound to be exceeded, if desired.

For example, if xlo = 2 and xhi = 12, then the x box length is 10 and the xy tilt factor must be between -5 and 5. Similarly, both xz and yz must be between -(xhi-xlo)/2 and +(yhi-ylo)/2. Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = . . . , -15, -5, 5, 15, 25, . . . are all equivalent.

To obey this constraint and allow for large shear deformations to be applied via the *xy*, *xz*, or *yz* parameters, the following algorithm is used. If *prd* is the associated parallel box length (10 in the example above), then if the tilt factor exceeds the accepted range of -5 to 5 during the simulation, then the box is flipped to the other limit (an equivalent box) and the simulation continues. Thus for this example, if the initial xy tilt factor was 0.0 and "xy final 100.0" was specified, then during the simulation the xy tilt factor would increase from 0.0 to 5.0, the box would be flipped so that the tilt factor becomes -5.0, the tilt factor would increase from -5.0 to 5.0, the box would be flipped again, etc. The flip occurs 10 times and the final tilt factor at the end of the simulation would be 0.0. During each flip event, atoms are remapped into the new box in the appropriate manner.

The one exception to this rule is if the 1st dimension in the tilt factor (x for xy) is non-periodic. In that case, the limits on the tilt factor are not enforced, since flipping the box in that dimension does not change the atom positions due to non-periodicity. In this mode, if you tilt the system to extreme angles, the simulation will simply become inefficient due to the highly skewed simulation box.

Each time the box size or shape is changed, the *remap* keyword determines whether atom positions are remapped to the new box. If *remap* is set to *x* (the default), atoms in the fix group are remapped; otherwise they are not. Note that their velocities are not changed, just their positions are altered. If *remap* is set to *v*, then any atom in the fix group that crosses a periodic boundary will have a delta added to its velocity equal to the difference in velocities between the lo and hi boundaries. Note that this velocity difference can include tilt components, e.g. a delta in the x velocity when an atom crosses the y periodic boundary. If *remap* is set to *none*, then neither of these remappings take place.

Conceptually, setting *remap* to *x* forces the atoms to deform via an affine transformation that exactly matches the box deformation. This setting is typically appropriate for solids. Note that though the atoms are effectively "moving" with the box over time, it is not due to their having a velocity that tracks the box change, but only due to the remapping. By contrast, setting *remap* to *v* is typically appropriate for fluids, where you want the atoms to respond to the change in box size/shape on their own and acquire a velocity that matches the box change, so that their motion will naturally track the box without explicit remapping of their coordinates.

Note: When non-equilibrium MD (NEMD) simulations are performed using this fix, the option "remap v" should normally be used. This is because *fix nvt/sllod* adjusts the atom positions and velocities to induce a velocity profile that matches the changing box size/shape. Thus atom coordinates should NOT be remapped by fix deform, but velocities

SHOULD be when atoms cross periodic boundaries, since that is consistent with maintaining the velocity profile already created by fix nvt/sllod. LAMMPS will warn you if the *remap* setting is not consistent with fix nvt/sllod.

Note: For non-equilibrium MD (NEMD) simulations using "remap v" it is usually desirable that the fluid (or flowing material, e.g. granular particles) stream with a velocity profile consistent with the deforming box. As mentioned above, using a thermostat such as *fix nvt/sllod* or *fix lavgevin* (with a bias provided by *compute temp/deform*), will typically accomplish that. If you do not use a thermostat, then there is no driving force pushing the atoms to flow in a manner consistent with the deforming box. E.g. for a shearing system the box deformation velocity may vary from 0 at the bottom to 10 at the top of the box. But the stream velocity profile of the atoms may vary from -5 at the bottom to +5 at the top. You can monitor these effects using the *fix ave/chunk*, *compute temp/deform*, and *compute temp/profile* commands. One way to induce atoms to stream consistent with the box deformation is to give them an initial velocity profile, via the *velocity ramp* command, that matches the box deformation rate. This also typically helps the system come to equilibrium more quickly, even if a thermostat is used.

Note: If a *fix rigid* is defined for rigid bodies, and *remap* is set to *x*, then the center-of-mass coordinates of rigid bodies will be remapped to the changing simulation box. This will be done regardless of whether atoms in the rigid bodies are in the fix deform group or not. The velocity of the centers of mass are not remapped even if *remap* is set to *v*, since *fix nvt/sllod* does not currently do anything special for rigid particles. If you wish to perform a NEMD simulation of rigid particles, you can either thermostat them independently or include a background fluid and thermostat the fluid via *fix nvt/sllod*.

The *flip* keyword allows the tilt factors for a triclinic box to exceed half the distance of the parallel box length, as discussed above. If the *flip* value is set to *yes*, the bound is enforced by flipping the box when it is exceeded. If the *flip* value is set to *no*, the tilt will continue to change without flipping. Note that if you apply large deformations, this means the box shape can tilt dramatically LAMMPS will run less efficiently, due to the large volume of communication needed to acquire ghost atoms around a processor's irregular-shaped sub-domain. For extreme values of tilt, LAMMPS may also lose atoms and generate an error.

The *units* keyword determines the meaning of the distance units used to define various arguments. A *box* value selects standard distance units as defined by the *units* command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacing. Note that the units choice also affects the *vel* style parameters since it is defined in terms of distance/time. Also note that the units keyword does not affect the *variable* style. You should use the *xlat*, *ylat*, *zlat* keywords of the *thermo_style* command if you want to include lattice spacings in a variable formula.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix will restore the initial box settings from *binary restart files*, which allows the fix to be properly continue deformation, when using the start/stop options of the *run* command. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*.

This fix can perform deformation over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.28.4 Restrictions

You cannot apply x, y, or z deformations to a dimension that is shrink-wrapped via the *boundary* command.

You cannot apply xy, yz, or xz deformations to a 2nd dimension (y in xy) that is shrink-wrapped via the *boundary* command.

16.28.5 Related commands

change_box

16.28.6 Default

The option defaults are remap = x, flip = yes, and units = lattice.

16.29 fix deposit command

16.29.1 Syntax

```
fix ID group-ID deposit N type M seed keyword values ...
```

- ID, group-ID are documented in *fix* command
- deposit = style name of this fix command
- N = # of atoms or molecules to insert
- type = atom type to assign to inserted atoms (offset for molecule insertion)
- M = insert a single atom or molecule every M steps
- seed = random # seed (positive integer)
- one or more keyword/value pairs may be appended to args
- keyword = *region* or *id* or *global* or *local* or *near* or *gaussian* or *attempt* or *rate* or *vx* or *vy* or *vz* or *mol* or *rigid* or *shake* or *units*

```
region value = region-ID
  region-ID = ID of region to use as insertion volume
id value = max or next
  max = atom ID for new atom(s) is max ID of all current atoms plus one
  next = atom ID for new atom(s) increments by one for every deposition
global values = lo hi
  lo,hi = put new atom/molecule a distance lo-hi above all other atoms␣
↪(distance units)
local values = lo hi delta
  lo,hi = put new atom/molecule a distance lo-hi above any nearby atom␣
↪beneath it (distance units)
```

```
    delta = lateral distance within which a neighbor is considered "nearby"␣
 ↪(distance units)
  near value = R
    R = only insert atom/molecule if further than R from existing particles␣
 ↪(distance units)
  gaussian values = xmid ymid zmid sigma
    xmid,ymid,zmid = center of the gaussian distribution (distance units)
    sigma = width of gaussian distribution (distance units)
  attempt value = Q
    Q = attempt a single insertion up to Q times
  rate value = V
    V = z velocity (y in 2d) at which insertion volume moves (velocity␣
 ↪units)
  vx values = vxlo vxhi
    vxlo,vxhi = range of x velocities for inserted atom/molecule (velocity␣
 ↪units)
  vy values = vylo vyhi
    vylo,vyhi = range of y velocities for inserted atom/molecule (velocity␣
 ↪units)
  vz values = vzlo vzhi
    vzlo,vzhi = range of z velocities for inserted atom/molecule (velocity␣
 ↪units)
  target values = tx ty tz
    tx,ty,tz = location of target point (distance units)
  mol value = template-ID
    template-ID = ID of molecule template specified in a separate molecule␣
 ↪command
  molfrac values = f1 f2 ... fN
    f1 to fN = relative probability of creating each of N molecules in␣
 ↪template-ID
  rigid value = fix-ID
    fix-ID = ID of fix rigid/small command
  shake value = fix-ID
    fix-ID = ID of fix shake command
  orient values = rx ry rz
    rx,ry,rz = vector to randomly rotate an inserted molecule around
  units value = lattice or box
    lattice = the geometry is defined in lattice units
    box = the geometry is defined in simulation box units
```

16.29.2 Examples

```
fix 3 all deposit 1000 2 100 29494 region myblock local 1.0 1.0 1.0 units box
fix 2 newatoms deposit 10000 1 500 12345 region disk near 2.0 vz -1.0 -0.8
fix 4 sputter deposit 1000 2 500 12235 region sphere vz -1.0 -1.0 target 5.0 5.0 0.0␣
 ↪units lattice
fix 5 insert deposit 200 2 100 777 region disk gaussian 5.0 5.0 9.0 1.0 units box
```

16.29.3 Description

Insert a single atom or molecule into the simulation domain every M timesteps until N atoms or molecules have been inserted. This is useful for simulating deposition onto a surface. For the remainder of this doc page, a single inserted atom or molecule is referred to as a "particle".

If inserted particles are individual atoms, they are assigned the specified atom type. If they are molecules, the type of each atom in the inserted molecule is specified in the file read by the *molecule* command, and those values are added to the specified atom type. E.g. if the file specifies atom types 1,2,3, and those are the atom types you want for inserted molecules, then specify *type* = 0. If you specify *type* = 2, the in the inserted molecule will have atom types 3,4,5.

All atoms in the inserted particle are assigned to two groups: the default group "all" and the group specified in the fix deposit command (which can also be "all").

If you are computing temperature values which include inserted particles, you will want to use the *compute_modify* dynamic option, which insures the current number of atoms is used as a normalizing factor each time the temperature is computed.

Care must be taken that inserted particles are not too near existing atoms, using the options described below. When inserting particles above a surface in a non-periodic box (see the *boundary* command), the possibility of a particle escaping the surface and flying upward should be considered, since the particle may be lost or the box size may grow infinitely large. A *fix wall/reflect* command can be used to prevent this behavior. Note that if a shrink-wrap boundary is used, it is OK to insert the new particle outside the box, however the box will immediately be expanded to include the new particle. When simulating a sputtering experiment it is probably more realistic to ignore those atoms using the *thermo_modify* command with the *lost ignore* option and a fixed *boundary*.

The fix deposit command must use the *region* keyword to define an insertion volume. The specified region must have been previously defined with a *region* command. It must be defined with side = *in*.

Note: LAMMPS checks that the specified region is wholly inside the simulation box. It can do this correctly for orthonormal simulation boxes. However for *triclinic boxes*, it only tests against the larger orthonormal box that bounds the tilted simulation box. If the specified region includes volume outside the tilted box, then an insertion will likely fail, leading to a "lost atoms" error. Thus for triclinic boxes you should insure the specified region is wholly inside the simulation box.

The locations of inserted particles are taken from uniform distributed random numbers, unless the *gaussian* keyword is used. Then the individual coordinates are taken from a gaussian distribution of width *sigma* centered on *xmid,ymid,zmid*.

Individual atoms are inserted, unless the *mol* keyword is used. It specifies a *template-ID* previously defined using the *molecule* command, which reads files that define one or more molecules. The coordinates, atom types, charges, etc, as well as any bond/angle/etc and special neighbor information for the molecule can be specified in the molecule file. See the *molecule* command for details. The only settings required to be in each file are the coordinates and types of atoms in the molecule.

If the molecule template contains more than one molecule, the relative probability of depositing each molecule can be specified by the *molfrac* keyword. N relative probabilities, each from 0.0 to 1.0, are specified, where N is the number of molecules in the template. Each time a molecule is deposited, a random number is used to sample from the list of relative probabilities. The N values must sum to 1.0.

If you wish to insert molecules via the *mol* keyword, that will be treated as rigid bodies, use the *rigid* keyword, specifying as its value the ID of a separate *fix rigid/small* command which also appears in your input script.

Note: If you wish the new rigid molecules (and other rigid molecules) to be thermostatted correctly via *fix rigid/small/nvt* or *fix rigid/small/npt*, then you need to use the "fix_modify dynamic/dof yes" command for the rigid

fix. This is to inform that fix that the molecule count will vary dynamically.

If you wish to insert molecules via the *mol* keyword, that will have their bonds or angles constrained via SHAKE, use the *shake* keyword, specifying as its value the ID of a separate *fix shake* command which also appears in your input script.

Each timestep a particle is inserted, the coordinates for its atoms are chosen as follows. For insertion of individual atoms, the "position" referred to in the following description is the coordinate of the atom. For insertion of molecule, the "position" is the geometric center of the molecule; see the *molecule* doc page for details. A random rotation of the molecule around its center point is performed, which determines the coordinates all the individual atoms.

A random position within the region insertion volume is generated. If neither the *global* or *local* keyword is used, the random position is the trial position. If the *global* keyword is used, the random x,y values are used, but the z position of the new particle is set above the highest current atom in the simulation by a distance randomly chosen between lo/hi. (For a 2d simulation, this is done for the y position.) If the *local* keyword is used, the z position is set a distance between lo/hi above the highest current atom in the simulation that is "nearby" the chosen x,y position. In this context, "nearby" means the lateral distance (in x,y) between the new and old particles is less than the *delta* setting.

Once a trial x,y,z position has been selected, the insertion is only performed if no current atom in the simulation is within a distance R of any atom in the new particle, including the effect of periodic boundary conditions if applicable. R is defined by the *near* keyword. Note that the default value for R is 0.0, which will allow atoms to strongly overlap if you are inserting where other atoms are present. This distance test is performed independently for each atom in an inserted molecule, based on the randomly rotated configuration of the molecule. If this test fails, a new random position within the insertion volume is chosen and another trial is made. Up to Q attempts are made. If the particle is not successfully inserted, LAMMPS prints a warning message.

Note: If you are inserting finite size particles or a molecule or rigid body consisting of finite-size particles, then you should typically set R larger than the distance at which any inserted particle may overlap with either a previously inserted particle or an existing particle. LAMMPS will issue a warning if R is smaller than this value, based on the radii of existing and inserted particles.

The *rate* option moves the insertion volume in the z direction (3d) or y direction (2d). This enables particles to be inserted from a successively higher height over time. Note that this parameter is ignored if the *global* or *local* keywords are used, since those options choose a z-coordinate for insertion independently.

The vx, vy, and vz components of velocity for the inserted particle are set using the values specified for the *vx*, *vy*, and *vz* keywords. Note that normally, new particles should be a assigned a negative vertical velocity so that they move towards the surface. For molecules, the same velocity is given to every particle (no rotation or bond vibration).

If the *target* option is used, the velocity vector of the inserted particle is changed so that it points from the insertion position towards the specified target point. The magnitude of the velocity is unchanged. This can be useful, for example, for simulating a sputtering process. E.g. the target point can be far away, so that all incident particles strike the surface as if they are in an incident beam of particles at a prescribed angle.

The *orient* keyword is only used when molecules are deposited. By default, each molecule is inserted at a random orientation. If this keyword is specified, then (rx,ry,rz) is used as an orientation vector, and each inserted molecule is rotated around that vector with a random value from zero to 2*PI. For a 2d simulation, rx = ry = 0.0 is required, since rotations can only be performed around the z axis.

The *id* keyword determines how atom IDs and molecule IDs are assigned to newly deposited particles. Molecule IDs are only assigned if molecules are being inserted. For the *max* setting, the atom and molecule IDs of all current atoms are checked. Atoms in the new particle are assigned IDs starting with the current maximum plus one. If a molecule is inserted it is assigned an ID = current maximum plus one. This means that if particles leave the system, the new IDs may replace the lost ones. For the *next* setting, the maximum ID of any atom and molecule is stored at the time the fix is defined. Each time a new particle is added, this value is incremented to assign IDs to the new atom(s) or molecule. Thus atom and molecule IDs for deposited particles will be consecutive even if particles leave the system over time.

The *units* keyword determines the meaning of the distance units used for the other deposition parameters. A *box* value selects standard distance units as defined by the *units* command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacing. Note that the units choice affects all the keyword values that have units of distance or velocity.

Note: If you are monitoring the temperature of a system where the atom count is changing due to adding particles, you typically should use the *compute_modify dynamic yes* command for the temperature compute you are using.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the deposition to *binary restart files*. This includes information about how many particles have been deposited, the random number generator seed, the next timestep for deposition, etc. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

Note: For this to work correctly, the timestep must **not** be changed after reading the restart with *reset_timestep*. The fix will try to detect it and stop with an error.

None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.29.4 Restrictions

This fix is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

The specified insertion region cannot be a "dynamic" region, as defined by the *region* command.

16.29.5 Related commands

fix pour, *region*

16.29.6 Default

Insertions are performed for individual atoms, i.e. no *mol* setting is defined. If the *mol* keyword is used, the default for *molfrac* is an equal probabilities for all molecules in the template. Additional option defaults are id = max, delta = 0.0, near = 0.0, attempt = 10, rate = 0.0, vx = 0.0 0.0, vy = 0.0 0.0, vz = 0.0 0.0, and units = lattice.

16.30 fix dpd/energy command

16.31 fix dpd/energy/kk command

16.31.1 Syntax

```
fix ID group-ID dpd/energy
```

- ID, group-ID are documented in *fix* command
- dpd/energy = style name of this fix command

16.31.2 Examples

```
fix 1 all dpd/energy
```

16.31.3 Description

Perform constant energy dissipative particle dynamics (DPD-E) integration. This fix updates the internal energies for particles in the group at each timestep. It must be used in conjunction with a deterministic integrator (e.g. *fix nve*) that updates the particle positions and velocities.

For fix *dpd/energy*, the particle internal temperature is related to the particle internal energy through a mesoparticle equation of state. An additional fix must be specified that defines the equation of state for each particle, e.g. *fix eos/cv*.

This fix must be used with the *pair_style dpd/fdt/energy* command.

Note that numerous variants of DPD can be specified by choosing an appropriate combination of the integrator and *pair_style dpd/fdt/energy* command. DPD under isoenergetic conditions can be specified by using fix *dpd/energy*, fix *nve* and pair_style *dpd/fdt/energy*. DPD under isoenthalpic conditions can be specified by using fix *dpd/energy*, fix *nph* and pair_style *dpd/fdt/energy*. Examples of each DPD variant are provided in the examples/USER/dpd directory.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

16.31.4 Restrictions

This command is part of the USER-DPD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix must be used with an additional fix that specifies time integration, e.g. *fix nve*.

The fix *dpd/energy* requires the *dpd atom_style* to be used in order to properly account for the particle internal energies and temperature.

The fix *dpd/energy* must be used with an additional fix that specifies the mesoparticle equation of state for each particle.

16.31.5 Related commands

fix nve *fix eos/cv*

Default: none

(Lisal) M. Lisal, J.K. Brennan, J. Bonet Avalos, "Dissipative particle dynamics at isothermal, isobaric, isoenergetic, and isoenthalpic conditions using Shardlow-like splitting algorithms.", J. Chem. Phys., 135, 204105 (2011).

(Larentzos) J.P. Larentzos, J.K. Brennan, J.D. Moore, and W.D. Mattson, "LAMMPS Implementation of Constant Energy Dissipative Particle Dynamics (DPD-E)", ARL-TR-6863, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD (2014).

16.32 fix edpd/source command

16.33 fix tdpd/source command

16.33.1 Syntax

```
fix ID group-ID edpd/source keyword values ...
fix ID group-ID tdpd/source cc_index keyword values ...
```

- ID, group-ID are documented in *fix* command
- edpd/source or tdpd/source = style name of this fix command
- index (only specified for tdpd/source) = index of chemical species (1 to Nspecies)
- keyword = *sphere* or *cuboid*

```
sphere values = cx,cy,cz,radius,source
  cx,cy,cz = x,y,z center of spherical domain (distance units)
  radius = radius of a spherical domain (distance units)
  source = heat source or concentration source (flux units, see below)
cuboid values = cx,cy,cz,dLx,dLy,dLz,source
  cx,cy,cz = x,y,z lower left corner of a cuboid domain (distance units)
  dLx,dLy,dLz = x,y,z side length of a cuboid domain (distance units)
  source = heat source or concentration source (flux units, see below)
```

16.33.2 Examples

```
fix 1 all edpd/source sphere 0.0 0.0 0.0 5.0 0.01
fix 1 all edpd/source cuboid 0.0 0.0 0.0 20.0 10.0 10.0 -0.01
fix 1 all tdpd/source 1 sphere 5.0 0.0 0.0 5.0 0.01
fix 1 all tdpd/source 2 cuboid 0.0 0.0 0.0 20.0 10.0 10.0 0.01
```

16.33.3 Description

Fix *edpd/source* adds a heat source as an external heat flux to each atom in a spherical or cuboid domain, where the *source* is in units of energy/time. Fix *tdpd/source* adds an external concentration source of the chemical species specified by *index* as an external concentration flux for each atom in a spherical or cuboid domain, where the *source* is in units of mole/volume/time.

This command can be used to give an additional heat/concentration source term to atoms in a simulation, such as for a simulation of a heat conduction with a source term (see Fig.12 in *(Li2014)*) or diffusion with a source term (see Fig.1 in *(Li2015)*), as an analog of a periodic Poiseuille flow problem.

If the *sphere* keyword is used, the *cx,cy,cz,radius* defines a spherical domain to apply the source flux to.

If the *cuboid* keyword is used, the *cx,cy,cz,dLx,dLy,dLz* defines a cuboid domain to apply the source flux to.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.33.4 Restrictions

This fix is part of the USER-MESO package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Fix *edpd/source* must be used with the *pair_style edpd* command. Fix *tdpd/source* must be used with the *pair_style tdpd* command.

16.33.5 Related commands

pair_style edpd, *pair_style tdpd*, *compute edpd/temp/atom*, *compute tdpd/cc/atom*

Default: none

(Li2014) Z. Li, Y.-H. Tang, H. Lei, B. Caswell and G.E. Karniadakis, "Energy-conserving dissipative particle dynamics with temperature-dependent properties", J. Comput. Phys., 265: 113-127 (2014). DOI: 10.1016/j.jcp.2014.02.003

(Li2015) Z. Li, A. Yazdani, A. Tartakovsky and G.E. Karniadakis, "Transport dissipative particle dynamics model for mesoscopic advection-diffusion-reaction problems", J. Chem. Phys., 143: 014101 (2015). DOI: 10.1063/1.4923254

16.34 fix drag command

16.34.1 Syntax

```
fix ID group-ID drag x y z fmag delta
```

- ID, group-ID are documented in *fix* command
- drag = style name of this fix command
- x,y,z = coord to drag atoms towards

- fmag = magnitude of force to apply to each atom (force units)
- delta = cutoff distance inside of which force is not applied (distance units)

16.34.2 Examples

```
fix center small-molecule drag 0.0 10.0 0.0 5.0 2.0
```

16.34.3 Description

Apply a force to each atom in a group to drag it towards the point (x,y,z). The magnitude of the force is specified by fmag. If an atom is closer than a distance delta to the point, then the force is not applied.

Any of the x,y,z values can be specified as NULL which means do not include that dimension in the distance calculation or force application.

This command can be used to steer one or more atoms to a new location in the simulation.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify* *respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix is adding its forces. Default is the outermost level.

This fix computes a global 3-vector of forces, which can be accessed by various *output commands*. This is the total force on the group of atoms by the drag force. The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.34.4 Restrictions

none

16.34.5 Related commands

fix spring, *fix spring/self*, *fix spring/rg*, *fix smd*

Default: none

16.35 fix drude command

16.35.1 Syntax

```
fix ID group-ID drude flag1 flag2 ... flagN
```

- ID, group-ID are documented in *fix* command
- drude = style name of this fix command
- flag1 flag2 ... flagN = Drude flag for each atom type (1 to N) in the system

16.35.2 Examples

```
fix 1 all drude 1 1 0 1 0 2 2 2
fix 1 all drude C C N C N D D D
```

16.35.3 Description

Assign each atom type in the system to be one of 3 kinds of atoms within the Drude polarization model. This fix is designed to be used with the *thermalized Drude oscillator model*. Polarizable models in LAMMPS are described on the *Howto polarizable* doc page.

The three possible types can be designated with an integer (0,1,2) or capital letter (N,C,D):

- 0 or N = non-polarizable atom (not part of Drude model)
- 1 or C = Drude core
- 2 or D = Drude electron

16.35.4 Restrictions

This fix should be invoked before any other commands that implement the Drude oscillator model, such as *fix langevin/drude*, *fix drude/transform*, *compute temp/drude*, *pair_style thole*.

16.35.5 Related commands

fix langevin/drude, *fix drude/transform*, *compute temp/drude*, *pair_style thole*

Default: None

16.36 fix drude/transform/direct command

16.37 fix drude/transform/inverse command

16.37.1 Syntax

```
fix ID group-ID style keyword value ...
```

- ID, group-ID are documented in *fix* command
- style = *drude/transform/direct* or *drude/transform/inverse*

16.37.2 Examples

```
fix 3 all drude/transform/direct
fix 1 all drude/transform/inverse
```

16.37.3 Description

Transform the coordinates of Drude oscillators from real to reduced and back for thermalizing the Drude oscillators as described in *(Lamoureux)* using a Nose-Hoover thermostat. This fix is designed to be used with the *thermalized Drude oscillator model*. Polarizable models in LAMMPS are described on the *Howto polarizable* doc page.

Drude oscillators are a pair of atoms representing a single polarizable atom. Ideally, the mass of Drude particles would vanish and their positions would be determined self-consistently by iterative minimization of the energy, the cores' positions being fixed. It is however more efficient and it yields comparable results, if the Drude oscillators (the motion of the Drude particle relative to the core) are thermalized at a low temperature. In that case, the Drude particles need a small mass.

The thermostats act on the reduced degrees of freedom, which are defined by the following equations. Note that in these equations upper case denotes atomic or center of mass values and lower case denotes Drude particle or dipole values. Primes denote the transformed (reduced) values, while bare letters denote the original values.

Masses:

$$M' = M + m$$

$$m' = \frac{M\,m}{M'}$$

Positions:

$$X' = \frac{M\,X + m\,x}{M'}$$

$$x' = x - X$$

Velocities:

$$V' = \frac{M\,V + m\,v}{M'}$$

$$v' = v - V$$

Forces:

$$F' = F + f$$

$$f' = \frac{M\,f - m\,F}{M'}$$

This transform conserves the total kinetic energy

$$\frac{1}{2}\,(M\,V^2\ + m\,v^2) = \frac{1}{2}\,(M'\,V'^2\ + m'\,v'^2)$$

and the virial defined with absolute positions

$$X\,F + x\,f = X'\,F' + x'\,f'$$

This fix requires each atom know whether it is a Drude particle or not. You must therefore use the *fix drude* command to specify the Drude status of each atom type.

Note: only the Drude core atoms need to be in the group specified for this fix. A Drude electron will be transformed together with its core even if it is not itself in the group. It is safe to include Drude electrons or non-polarizable atoms in the group. The non-polarizable atoms will simply not be transformed.

This fix does NOT perform time integration. It only transform masses, coordinates, velocities and forces. Thus you must use separate time integration fixes, like *fix nve* or *fix npt* to actually update the velocities and positions of atoms. In order to thermalize the reduced degrees of freedom at different temperatures, two Nose-Hoover thermostats must be defined, acting on two distinct groups.

Note: The *fix drude/transform/direct* command must appear before any Nose-Hoover thermostatting fixes. The *fix drude/transform/inverse* command must appear after any Nose-Hoover thermostatting fixes.

Example:

```
fix fDIRECT all drude/transform/direct
fix fNVT gCORES nvt temp 300.0 300.0 100
fix fNVT gDRUDES nvt temp 1.0 1.0 100
fix fINVERSE all drude/transform/inverse
compute TDRUDE all temp/drude
thermo_style custom step cpu etotal ke pe ebond ecoul elong press vol temp c_
↪TDRUDE[1] c_TDRUDE[2]
```

In this example, *gCORES* is the group of the atom cores and *gDRUDES* is the group of the Drude particles (electrons). The centers of mass of the Drude oscillators will be thermostatted at 300.0 and the internal degrees of freedom will be thermostatted at 1.0. The temperatures of cores and Drude particles, in center-of-mass and relative coordinates, are calculated using *compute temp/drude*

In addition, if you want to use a barostat to simulate a system at constant pressure, only one of the Nose-Hoover fixes must be *npt*, the other one should be *nvt*. You must add a *compute temp/com* and a *fix_modify* command so that the temperature of the *npt* fix be just that of its group (the Drude cores) but the pressure be the overall pressure *thermo_press*.

Example:

```
compute cTEMP_CORE gCORES temp/com
fix fDIRECT all drude/transform/direct
fix fNPT gCORES npt temp 298.0 298.0 100 iso 1.0 1.0 500
fix_modify fNPT temp cTEMP_CORE press thermo_press
fix fNVT gDRUDES nvt temp 5.0 5.0 100
fix fINVERSE all drude/transform/inverse
```

In this example, *gCORES* is the group of the atom cores and *gDRUDES* is the group of the Drude particles. The centers of mass of the Drude oscillators will be thermostatted at 298.0 and the internal degrees of freedom will be thermostatted at 5.0. The whole system will be barostatted at 1.0.

In order to avoid the flying ice cube problem (irreversible transfer of linear momentum to the center of mass of the system), you may need to add a *fix momentum* command:

```
fix fMOMENTUM all momentum 100 linear 1 1 1
```

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

16.37.4 Restrictions

none

16.37.5 Related commands

fix drude, *fix langevin/drude*, *compute temp/drude*, *pair_style thole*

Default: none

(Lamoureux) Lamoureux and Roux, J Chem Phys, 119, 3025-3039 (2003).

16.38 fix dt/reset command

16.38.1 Syntax

```
fix ID group-ID dt/reset N Tmin Tmax Xmax keyword values ...
```

- ID, group-ID are documented in *fix* command
- dt/reset = style name of this fix command
- N = re-compute dt every N timesteps
- Tmin = minimum dt allowed which can be NULL (time units)
- Tmax = maximum dt allowed which can be NULL (time units)
- Xmax = maximum distance for an atom to move in one timestep (distance units)
- zero or more keyword/value pairs may be appended
- keyword = *emax* or *units*

```
emax value = Emax
  Emax = maximum kinetic energy change for an atom in one timestep (energy␣
↪units)
units value = lattice or box
  lattice = Xmax is defined in lattice units
  box = Xmax is defined in simulation box units
```

16.38.2 Examples

```
fix 5 all dt/reset 10 1.0e-5 0.01 0.1
fix 5 all dt/reset 10 0.01 2.0 0.2 units box
fix 5 all dt/reset 5 NULL 0.001 0.5 emax 30 units box
```

16.38.3 Description

Reset the timestep size every N steps during a run, so that no atom moves further than the specified *Xmax* distance, based on current atom velocities and forces. Optionally an additional criterion is imposed by the *emax* keyword, so that no atom's kinetic energy changes by more than the specified *Emax*.

This can be useful when starting from a configuration with overlapping atoms, where forces will be large. Or it can be useful when running an impact simulation where one or more high-energy atoms collide with a solid, causing a damage cascade.

This fix overrides the timestep size setting made by the *timestep* command. The new timestep size *dt* is computed in the following manner.

For each atom, the timestep is computed that would cause it to displace *Xmax* on the next integration step, as a function of its current velocity and force. Since performing this calculation exactly would require the solution to a quartic equation, a cheaper estimate is generated. The estimate is conservative in that the atom's displacement is guaranteed not to exceed *Xmax*, though it may be smaller.

In addition if the *emax* keyword is used, the specified *Emax* value is enforced as a limit on how much an atom's kinetic energy can change. If the timestep required is even smaller than for the *Xmax* displacement, then the smaller timestep is used.

Given this putative timestep for each atom, the minimum timestep value across all atoms is computed. Then the *Tmin* and *Tmax* bounds are applied, if specified. If one (or both) is specified as NULL, it is not applied.

When the *run style* is *respa*, this fix resets the outer loop (largest) timestep, which is the same timestep that the *timestep* command sets.

Note that the cumulative simulation time (in time units), which accounts for changes in the timestep size as a simulation proceeds, can be accessed by the *thermo_style time* keyword.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix computes a global scalar which can be accessed by various *output commands*. The scalar stores the last timestep on which the timestep was reset to a new value.

The scalar value calculated by this fix is "intensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.38.4 Restrictions

none

16.38.5 Related commands

timestep

16.38.6 Default

The option defaults are units = lattice, and no emax kinetic energy limit.

16.39 fix efield command

16.39.1 Syntax

```
fix ID group-ID efield ex ey ez keyword value ...
```

- ID, group-ID are documented in *fix* command
- efield = style name of this fix command
- ex,ey,ez = E-field component values (electric field units)
- any of ex,ey,ez can be a variable (see below)
- zero or more keyword/value pairs may be appended to args
- keyword = *region* or *energy*

```
region value = region-ID
  region-ID = ID of region atoms must be in to have added force
energy value = v_name
  v_name = variable with name that calculates the potential energy of␣
↪each atom in the added E-field
```

16.39.2 Examples

```
fix kick external-field efield 1.0 0.0 0.0
fix kick external-field efield 0.0 0.0 v_oscillate
```

16.39.3 Description

Add a force F = qE to each charged atom in the group due to an external electric field being applied to the system. If the system contains point-dipoles, also add a torque on the dipoles due to the external electric field.

For charges, any of the 3 quantities defining the E-field components can be specified as an equal-style or atom-style *variable*, namely *ex*, *ey*, *ez*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the E-field component.

For point-dipoles, equal-style variables can be used, but atom-style variables are not currently supported, since they imply a spatial gradient in the electric field which means additional terms with gradients of the field are required for the force and torque on dipoles.

Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent E-field.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent E-field with optional time-dependence as well.

If the *region* keyword is used, the atom must also be in the specified geometric *region* in order to have force added to it.

Adding a force or torque to atoms implies a change in their potential energy as they move or rotate due to the applied E-field.

For dynamics via the "run" command, this energy can be optionally added to the system's potential energy for thermodynamic output (see below). For energy minimization via the "minimize" command, this energy must be added to the system's potential energy to formulate a self-consistent minimization problem (see below).

The *energy* keyword is not allowed if the added field is a constant vector (ex,ey,ez), with all components defined as numeric constants and not as variables. This is because LAMMPS can compute the energy for each charged particle directly as E = -x dot qE = -q (x*ex + y*ey + z*ez), so that -Grad(E) = F. Similarly for point-dipole particles the energy can be computed as E = -mu dot E = -(mux*ex + muy*ey + muz*ez).

The *energy* keyword is optional if the added force is defined with one or more variables, and if you are performing dynamics via the *run* command. If the keyword is not used, LAMMPS will set the energy to 0.0, which is typically fine for dynamics.

The *energy* keyword is required if the added force is defined with one or more variables, and you are performing energy minimization via the "minimize" command for charged particles. It is not required for point-dipoles, but a warning is issued since the minimizer in LAMMPS does not rotate dipoles, so you should not expect to be able to minimize the orientation of dipoles in an applied electric field.

The *energy* keyword specifies the name of an atom-style *variable* which is used to compute the energy of each atom as function of its position. Like variables used for *ex*, *ey*, *ez*, the energy variable is specified as v_name, where name is the variable name.

Note that when the *energy* keyword is used during an energy minimization, you must insure that the formula defined for the atom-style *variable* is consistent with the force variable formulas, i.e. that -Grad(E) = F. For example, if the force due to the electric field were a spring-like F = kx, then the energy formula should be E = -0.5kx^2. If you don't do this correctly, the minimization will not converge properly.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify* *energy* option is supported by this fix to add the potential "energy" inferred by the added force due to the electric field to the system's potential energy as part of *thermodynamic output*. This is a fictitious quantity but is needed so that the *minimize* command can include the forces added by this fix in a consistent manner. I.e. there is a decrease in potential energy when atoms move in the direction of the added force due to the electric field.

The *fix_modify* *virial* option is supported by this fix to add the contribution due to the added forces on atoms to the system's virial as part of *thermodynamic output*. The default is *virial no*

The *fix_modify* *respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix adding its forces. Default is the outermost level.

This fix computes a global scalar and a global 3-vector of forces, which can be accessed by various *output commands*. The scalar is the potential energy discussed above. The vector is the total force added to the group of atoms. The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command. You should not specify force components with a variable that has time-dependence for use with a minimizer, since the minimizer increments the timestep as the iteration count during the minimization.

Note: If you want the fictitious potential energy associated with the added forces to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the *fix_modify* *energy* option for this fix.

16.39.4 Restrictions

This fix is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.39.5 Related commands

fix addforce

Default: none

16.40 fix ehex command

16.40.1 Syntax

```
fix ID group-ID ehex nevery F keyword value
```

- ID, group-ID are documented in *fix* command
- ehex = style name of this fix command
- nevery = add/subtract heat every this many timesteps
- F = energy flux into the reservoir (energy/time units)
- zero or more keyword/value pairs may be appended to args
- keyword = *region* or *constrain* or *com* or *hex*

```
region value = region-ID
  region-ID = ID of region (reservoir) atoms must be in for added␣
↪thermostatting force
constrain value = none
  apply the constraint algorithm (SHAKE or RATTLE) again at the end of␣
↪the timestep
com value = none
  rescale all sites of a constrained cluster of atom if its COM is in the␣
↪reservoir
hex value = none
  omit the coordinate correction to recover the HEX algorithm
```

16.40.2 Examples

```
# Lennard-Jones, from examples/in.ehex.lj

fix fnve all nve
# specify regions rhot and rcold
...
fix fhot all ehex 1 0.15 region rhot
fix fcold all ehex 1 -0.15 region rcold

# SPC/E water, from examples/in.ehex.spce
fix fnve all nve
# specify regions rhot and rcold
...
fix fhot all ehex 1 0.075 region rhot constrain com
fix fcold all ehex 1 -0.075 region rcold constrain com
fix frattle all rattle 1e-10 400 0 b 1 a 1
```

16.40.3 Description

This fix implements the asymmetric version of the enhanced heat exchange algorithm *(Wirnsberger)*. The eHEX algorithm is an extension of the heat exchange algorithm *(Ikeshoji)* and adds an additional coordinate integration to account for higher-order truncation terms in the operator splitting. The original HEX algorithm (implemented as *fix heat*) is known to exhibit a slight energy drift limiting the accessible simulation times to a few nanoseconds. This issue is greatly improved by the new algorithm decreasing the energy drift by at least a factor of a hundred (LJ and SPC/E water) with little computational overhead.

In both algorithms (non-translational) kinetic energy is constantly swapped between regions (reservoirs) to impose a heat flux onto the system. The equations of motion are therefore modified if a particle i is located inside a reservoir Γ_k where $k > 0$. We use Γ_0 to label those parts of the simulation box which are not thermostatted.) The input parameter *region-ID* of this fix corresponds to k. The energy swap is modelled by introducing an additional thermostatting force to the equations of motion, such that the time evolution of coordinates and momenta of particle i becomes *(Wirnsberger)*

$$\dot{\mathbf{r}}_i = \mathbf{v}_i,$$
$$\dot{\mathbf{v}}_i = \frac{\mathbf{f}_i}{m_i} + \frac{\mathbf{g}_i}{m_i}.$$

The thermostatting force is given by

$$\mathbf{g}_i = \begin{cases} \frac{m_i}{2} \frac{F_{\Gamma_{k(\mathbf{r}_i)}}}{K_{\Gamma_{k(\mathbf{r}_i)}}} \left(\mathbf{v}_i - \mathbf{v}_{\Gamma_{k(\mathbf{r}_i)}}\right) & k(\mathbf{r}_i) > 0 \text{ (inside a reservoir)}, \\ 0 & \text{otherwise}, \end{cases}$$

where m_i is the mass and $k(\mathbf{r}_i)$ maps the particle position to the respective reservoir. The quantity $F_{\Gamma_{k(\mathbf{r}_i)}}$ corresponds to the input parameter F, which is the energy flux into the reservoir. Furthermore, $K_{\Gamma_{k(\mathbf{r}_i)}}$ and $v_{\Gamma_{k(\mathbf{r}_i)}}$ denote the non-translational kinetic energy and the center of mass velocity of that reservoir. The thermostatting force does not affect the center of mass velocities of the individual reservoirs and the entire simulation box. A derivation of the equations and details on the numerical implementation with velocity Verlet in LAMMPS can be found in reference "(Wirnsberger)"#_Wirnsberger.

Note: This fix only integrates the thermostatting force and must be combined with another integrator, such as *fix nve*, to solve the full equations of motion.

This fix is different from a thermostat such as *fix nvt* or *fix temp/rescale* in that energy is added/subtracted continually. Thus if there isn't another mechanism in place to counterbalance this effect, the entire system will heat or cool continuously.

Note: If heat is subtracted from the system too aggressively so that the group's kinetic energy would go to zero, then LAMMPS will halt with an error message. Increasing the value of *nevery* means that heat is added/subtracted less frequently but in larger portions. The resulting temperature profile will therefore be the same.

This fix will default to *fix_heat* (HEX algorithm) if the keyword *hex* is specified.

Compatibility with SHAKE and RATTLE (rigid molecules):

This fix is compatible with *fix shake* and *fix rattle*. If either of these constraining algorithms is specified in the input script and the keyword *constrain* is set, the bond distances will be corrected a second time at the end of the integration step. It is recommended to specify the keyword *com* in addition to the keyword *constrain*. With this option all sites of a constrained cluster are rescaled, if its center of mass is located inside the region. Rescaling all sites of a cluster by the same factor does not introduce any velocity components along fixed bonds. No rescaling takes place if the center of mass lies outside the region.

Note: You can only use the keyword *com* along with *constrain*.

To achieve the highest accuracy it is recommended to use *fix rattle* with the keywords *constrain* and *com* as shown in the second example. Only if RATTLE is employed, the velocity constraints will be satisfied.

Note: Even if RATTLE is used and the keywords *com* and *constrain* are both set, the coordinate constraints will not necessarily be satisfied up to the target precision. The velocity constraints are satisfied as long as all sites of a cluster are rescaled (keyword *com*) and the cluster does not span adjacent reservoirs. The current implementation of the eHEX algorithm introduces a small error in the bond distances, which goes to zero with order three in the timestep. For example, in a simulation of SPC/E water with a timestep of 2 fs the maximum relative error in the bond distances was found to be on the order of 10^{-7} for relatively large temperature gradients. A higher precision can be achieved by decreasing the timestep.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.40.4 Restrictions

This fix is part of the RIGID package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.40.5 Related commands

fix heat, *fix thermal/conductivity*, *compute temp*, *compute temp/region*

Default: none

(Ikeshoji) Ikeshoji and Hafskjold, Molecular Physics, 81, 251-261 (1994).

(Wirnsberger) Wirnsberger, Frenkel, and Dellago, J Chem Phys, 143, 124104 (2015).

16.41 fix electron/stopping command

16.41.1 Syntax

```
fix ID group-ID electron/stopping Ecut file keyword value ...
```

- ID, group-ID are documented in *fix* command
- electron/stopping = style name of this fix command
- Ecut = minimum kinetic energy for electronic stopping (energy units)
- file = name of the file containing the electronic stopping power table
- zero or more keyword/value pairs may be appended to args
- keyword = *region* or *minneigh*

```
region value = region-ID
  region-ID = region, whose atoms will be affected by this fix
minneigh value = minneigh
  minneigh = minimum number of neighbors an atom to have stopping applied
```

16.41.2 Examples

```
fix el all electron/stopping 10.0 elstop-table.txt
fix el all electron/stopping 10.0 elstop-table.txt minneigh 3
fix el mygroup electron/stopping 1.0 elstop-table.txt region bulk
```

16.41.3 Description

This fix implements inelastic energy loss for fast projectiles in solids. It applies a friction force to fast moving atoms to slow them down due to *electronic stopping* (energy lost via electronic collisions per unit of distance). This fix should be used for simulation of irradiation damage or ion implantation, where the ions can lose noticeable amounts of energy from electron excitations. If the electronic stopping power is not considered, the simulated range of the ions can be severely overestimated (*Nordlund98*, *Nordlund95*).

The electronic stopping is implemented by applying a friction force to each atom as:

$$\vec{F}_i = \vec{F}_i^0 - \frac{\vec{v}_i}{\|\vec{v}_i\|} \cdot S_e$$

where $\vec{F}_i$ is the resulting total force on the atom. $\vec{F}_i^0$ is the original force applied to the atom, $\vec{v}_i$ is its velocity and S_e is the stopping power of the ion.

Note: In addition to electronic stopping, atomic cascades and irradiation simulations require the use of an adaptive timestep (see *fix dt/reset*) and the repulsive ZBL potential (see *ZBL* potential) or similar. Without these settings the interaction between the ion and the target atoms will be faulty. It is also common to use in such simulations a thermostat (*fix_nvt*) in the borders of the simulation cell.

Note: This fix removes energy from fast projectiles without depositing it as a heat to the simulation cell. Such implementation might lead to the unphysical results when the amount of energy deposited to the electronic system is large, e.g. simulations of Swift Heavy Ions (energy per nucleon of 100 keV/amu or higher) or multiple projectiles. You could compensate energy loss by coupling bulk atoms with some thermostat or control heat transfer between electronic and atomic subsystems with the two-temperature model (*fix_ttm*).

At low velocities the electronic stopping is negligible. The electronic friction is not applied to atoms whose kinetic energy is smaller than *Ecut*, or smaller than the lowest energy value given in the table in *file*. Electronic stopping should be applied only when a projectile reaches bulk material. This fix scans neighbor list and excludes atoms with fewer than *minneigh* neighbors (by default one). If the pair potential cutoff is large, minneigh should be increased, though not above the number of nearest neighbors in bulk material. An alternative is to disable the check for neighbors by setting *minneigh* to zero and using the *region* keyword. This is necessary when running simulations of cluster bombardment.

If the *region* keyword is used, the atom must also be in the specified geometric *region* in order to have electronic stopping applied to it. This is useful if the position of the bulk material is fixed. By default the electronic stopping is applied everywhere in the simulation cell.

The energy ranges and stopping powers are read from the file *file*. Lines starting with # and empty lines are ignored. Otherwise each line must contain exactly **N+1** numbers, where **N** is the number of atom types in the simulation.

The first column is the energy for which the stopping powers on that line apply. The energies must be sorted from the smallest to the largest. The other columns are the stopping powers S_e for each atom type, in ascending order, in force *units*. The stopping powers for intermediate energy values are calculated with linear interpolation between 2 nearest points.

For example:

```
# This is a comment
#       atom-1    atom-2
# eV    eV/Ang    eV/Ang  # units metal
 10        0        0
250       60       80
750      100      150
```

If an atom which would have electronic stopping applied to it has a kinetic energy higher than the largest energy given in *file*, LAMMPS will exit with an error message.

The stopping power depends on the energy of the ion and the target material. The electronic stopping table can be obtained from scientific publications, experimental databases or by using *SRIM* software. Other programs such as *CasP* or *PASS* can calculate the energy deposited as a function of the impact parameter of the ion; these results can be used to derive the stopping power.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify* options are not supported.

This fix computes a global scalar, which can be accessed by various *output commands*. The scalar is the total energy loss from electronic stopping applied by this fix since the start of the latest run. It is considered "intensive".

The *start/stop* keywords of the *run* command have no effect on this fix.

16.41.4 Restrictions

This pair style is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.41.5 Default

The default is no limitation by region, and minneigh = 1.

(electronic stopping) Wikipedia - Electronic Stopping Power: https://en.wikipedia.org/wiki/Stopping_power_%28particle_radiation%29

(Nordlund98) Nordlund, Kai, et al. Physical Review B 57.13 (1998): 7556.

(Nordlund95) Nordlund, Kai. Computational materials science 3.4 (1995): 448-456.

(SRIM) SRIM webpage: http://www.srim.org/

(CasP) CasP webpage: https://www.helmholtz-berlin.de/people/gregor-schiwietz/casp_en.html

(PASS) PASS webpage: https://www.sdu.dk/en/DPASS

16.42 fix enforce2d command

16.43 fix enforce2d/kk command

16.43.1 Syntax

```
fix ID group-ID enforce2d
```

- ID, group-ID are documented in *fix* command
- enforce2d = style name of this fix command

16.43.2 Examples

```
fix 5 all enforce2d
```

16.43.3 Description

Zero out the z-dimension velocity and force on each atom in the group. This is useful when running a 2d simulation to insure that atoms do not move from their initial z coordinate.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command.

16.43.4 Restrictions

none

Related commands: none

Default: none

16.44 fix eos/cv command

16.44.1 Syntax

```
fix ID group-ID eos/cv cv
```

- ID, group-ID are documented in *fix* command
- eos/cv = style name of this fix command
- cv = constant-volume heat capacity (energy/temperature units)

16.44.2 Examples

```
fix 1 all eos/cv 0.01
```

16.44.3 Description

Fix *eos/cv* applies a mesoparticle equation of state to relate the particle internal energy (u_i) to the particle internal temperature (θ_i). The *eos/cv* mesoparticle equation of state requires the constant-volume heat capacity, and is defined as follows:

$$u_i = u_i^{mech} + u_i^{cond} = C_V \theta_i$$

where C_V is the constant-volume heat capacity, u^{cond} is the internal conductive energy, and u^{mech} is the internal mechanical energy. Note that alternative definitions of the mesoparticle equation of state are possible.

16.44.4 Restrictions

This command is part of the USER-DPD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This command also requires use of the *atom_style dpd* command.

16.44.5 Related commands

fix shardlow, *pair dpd/fdt*

Default: none

(Larentzos) J.P. Larentzos, J.K. Brennan, J.D. Moore, and W.D. Mattson, "LAMMPS Implementation of Constant Energy Dissipative Particle Dynamics (DPD-E)", ARL-TR-6863, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD (2014).

16.45 fix eos/table command

16.45.1 Syntax

```
fix ID group-ID eos/table style file N keyword
```

- ID, group-ID are documented in *fix* command
- eos/table = style name of this fix command
- style = *linear* = method of interpolation
- file = filename containing the tabulated equation of state
- N = use N values in *linear* tables
- keyword = name of table keyword corresponding to table file

16.45.2 Examples

```
fix 1 all eos/table linear eos.table 100000 KEYWORD
```

16.45.3 Description

Fix *eos/table* applies a tabulated mesoparticle equation of state to relate the particle internal energy (u_i) to the particle internal temperature (dpdTheta_i).

Fix *eos/table* creates interpolation tables of length *N* from internal energy values listed in a file as a function of internal temperature.

The interpolation tables are created by fitting cubic splines to the file values and interpolating energy values at each of *N* internal temperatures, and vice versa. During a simulation, these tables are used to interpolate internal energy or temperature values as needed. The interpolation is done with the *linear* style.

For the *linear* style, the internal temperature is used to find 2 surrounding table values from which an internal energy is computed by linear interpolation, and vice versa.

The filename specifies a file containing tabulated internal temperature and internal energy values. The keyword specifies a section of the file. The format of this file is described below.

The format of a tabulated file is as follows (without the parenthesized comments):

```
# EOS TABLE                 (one or more comment or blank lines)

KEYWORD                     (keyword is first text on line)
N 500                       (N  parameter)
                            (blank)
1   1.00 0.000              (index, internal temperature, internal energy)
2   1.02 0.001
...
500 10.0 0.500
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the fix command.

The next line lists the number of table entries. The parameter "N" is required and its value is the number of table entries that follow. Note that this may be different than the *N* specified in the *fix eos/table* command. Let Ntable = *N* in the fix command, and Nfile = "N" in the tabulated file. What LAMMPS does is a preliminary interpolation by creating splines using the Nfile tabulated values as nodal points. It uses these to interpolate as needed to generate energy and temperature values at Ntable different points. The resulting tables of length Ntable are then used as described above, when computing energy and temperature relationships. This means that if you want the interpolation tables of length Ntable to match exactly what is in the tabulated file (with effectively no preliminary interpolation), you should set Ntable = Nfile.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is the internal temperature (in temperature units), the 3rd value is the internal energy (in energy units).

Note that the internal temperature and internal energy values must increase from one line to the next.

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

16.45.4 Restrictions

This command is part of the USER-DPD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This command also requires use of the *atom_style dpd* command.

The equation of state must be a monotonically increasing function.

An error will occur if the internal temperature or internal energies are not within the table cutoffs.

16.45.5 Related commands

fix shardlow, *pair dpd/fdt*

Default: none

16.46 fix eos/table/rx command

16.47 fix eos/table/rx/kk command

16.47.1 Syntax

```
fix ID group-ID eos/table/rx style file1 N keyword ...
```

- ID, group-ID are documented in *fix* command
- eos/table/rx = style name of this fix command
- style = *linear* = method of interpolation
- file1 = filename containing the tabulated equation of state
- N = use N values in *linear* tables
- keyword = name of table keyword corresponding to table file
- file2 = filename containing the heats of formation of each species (optional)
- deltaHf = heat of formation for a single species in energy units (optional)
- energyCorr = energy correction in energy units (optional)
- tempCorrCoeff = temperature correction coefficient (optional)

16.47.2 Examples

```
fix 1 all eos/table/rx linear eos.table 10000 KEYWORD thermo.table
fix 1 all eos/table/rx linear eos.table 10000 KEYWORD 1.5
fix 1 all eos/table/rx linear eos.table 10000 KEYWORD 1.5 0.025 0.0
```

16.47.3 Description

Fix *eos/table/rx* applies a tabulated mesoparticle equation of state to relate the concentration-dependent particle internal energy (u_i) to the particle internal temperature (θ_i).

The concentration-dependent particle internal energy (u_i) is computed according to the following relation:

$$U_i = \sum_{j=1}^{m} c_{i,j}(u_j + \Delta H_{f,j}) + \frac{3k_bT}{2} + Nk_bT$$

where *m* is the number of species, $c_{i,j}$ is the concentration of species *j* in particle *i*, u_j is the internal energy of species j, $\Delta H_{f,j} istheheatofformationofspecies*j*, Nisthenumberofmoleculesrepresentedbythecoarse-grainedparticle,: math$: is the Boltzmann constant, and *T* is the temperature of the system. Additionally, it is possible to modify the concentration-dependent particle internal energy relation by adding an energy correction, temperature-dependent correction, and/or a molecule-dependent correction. An energy correction can be specified as a constant (in energy units). A temperature correction can be specified by multiplying a temperature correction coefficient by the internal temperature. A molecular correction can be specified by by multiplying a molecule correction coefficient by the average number of product gas particles in the coarse-grain particle.

Fix *eos/table/rx* creates interpolation tables of length *N* from *m* internal energy values of each species u_j listed in a file as a function of internal temperature. During a simulation, these tables are used to interpolate internal energy or temperature values as needed. The interpolation is done with the *linear* style. For the *linear* style, the internal temperature is used to find 2 surrounding table values from which an internal energy is computed by linear interpolation. A secant solver is used to determine the internal temperature from the internal energy.

The first filename specifies a file containing tabulated internal temperature and *m* internal energy values for each species u_j. The keyword specifies a section of the file. The format of this file is described below.

The second filename specifies a file containing heat of formation $\Delta H_{f,j}$ for each species.

In cases where the coarse-grain particle represents a single molecular species (i.e., no reactions occur and fix *rx* is not present in the input file), fix *eos/table/rx* can be applied in a similar manner to fix *eos/table* within a non-reactive DPD simulation. In this case, the heat of formation filename is replaced with the heat of formation value for the single species. Additionally, the energy correction and temperature correction coefficients may also be specified as fix arguments.

The format of a tabulated file is as follows (without the parenthesized comments):

```
# EOS TABLE                 (one or more comment or blank lines)

KEYWORD                     (keyword is first text on line)
N 500 h2 no2 n2 ... no      (N  parameter species1 species2 ... speciesN)
                            (blank)
1   1.00 0.000 ... 0.0000   (index, internal temperature, internal energy of species 1,
↪ ..., internal energy of species m)
2   1.02 0.001 ... 0.0002
...
500 10.0 0.500 ... 1.0000
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the fix command.

The next line lists the number of table entries and the species names that correspond with all the species listed in the reaction equations through the *fix rx* command. The parameter "N" is required and its value is the number of table entries that follow. Let Nfile = "N" in the tabulated file. What LAMMPS does is a preliminary interpolation by creating splines using the Nfile tabulated values as nodal points.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is the internal temperature (in temperature units), the 3rd value until the *m+3* value are the internal energies of the m species (in energy units).

Note that all internal temperature and internal energy values must increase from one line to the next.

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

The format of a heat of formation file is as follows (without the parenthesized comments):

```
# HEAT OF FORMATION TABLE  (one or more comment or blank lines)

                           (blank)
h2      0.00               (species name, heat of formation)
no2     0.34
n2      0.00
...
no      0.93
```

Note that the species can be listed in any order. The tag that is used as the species name must correspond with the tags used to define the reactions with the *fix rx* command.

Alternatively, corrections to the EOS can be included by specifying three additional columns that correspond to the energy correction, the temperature correction coefficient and molecule correction coefficient. In this case, the format of the file is as follows:

```
# HEAT OF FORMATION TABLE     (one or more comment or blank lines)

                              (blank)
h2      0.00 1.23 0.025  0.0  (species name, heat of formation, energy correction,␣
↪temperature correction coefficient, molecule correction coefficient)
no2     0.34 0.00 0.000 -1.76
n2      0.00 0.00 0.000 -1.76
...
no      0.93 0.00 0.000 -1.76
```

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

16.47.4 Restrictions

This command is part of the USER-DPD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This command also requires use of the *atom_style dpd* command.

The equation of state must be a monotonically increasing function.

An error will occur if the internal temperature or internal energies are not within the table cutoffs.

16.47.5 Related commands

fix rx, *pair dpd/fdt*

Default: none

16.48 fix evaporate command

16.48.1 Syntax

```
fix ID group-ID evaporate N M region-ID seed
```

- ID, group-ID are documented in *fix* command
- evaporate = style name of this fix command
- N = delete atoms every this many timesteps
- M = number of atoms to delete each time
- region-ID = ID of region within which to perform deletions
- seed = random number seed to use for choosing atoms to delete
- zero or more keyword/value pairs may be appended

  ```
  keyword = molecule
    molecule value = no or yes
  ```

16.48.2 Examples

```
fix 1 solvent evaporate 1000 10 surface 49892
fix 1 solvent evaporate 1000 10 surface 38277 molecule yes
```

16.48.3 Description

Remove M atoms from the simulation every N steps. This can be used, for example, to model evaporation of solvent particles or molecules (i.e. drying) of a system. Every N steps, the number of atoms in the fix group and within the specified region are counted. M of these are chosen at random and deleted. If there are less than M eligible particles, then all of them are deleted.

If the setting for the *molecule* keyword is *no*, then only single atoms are deleted. In this case, you should insure you do not delete only a portion of a molecule (only some of its atoms), or LAMMPS will soon generate an error when it tries to find those atoms. LAMMPS will warn you if any of the atoms eligible for deletion have a non-zero molecule ID, but does not check for this at the time of deletion.

If the setting for the *molecule* keyword is *yes*, then when an atom is chosen for deletion, the entire molecule it is part of is deleted. The count of deleted atoms is incremented by the number of atoms in the molecule, which may make it exceed *M*. If the molecule ID of the chosen atom is 0, then it is assumed to not be part of a molecule, and just the single atom is deleted.

As an example, if you wish to delete 10 water molecules every *N* steps, you should set *M* to 30. If only the water's oxygen atoms were in the fix group, then two hydrogen atoms would be deleted when an oxygen atom is selected for deletion, whether the hydrogen atoms are inside the evaporation region or not.

Note that neighbor lists are re-built on timesteps that atoms are removed. Thus you should not remove atoms too frequently or you will incur overhead due to the cost of building neighbor lists.

Note: If you are monitoring the temperature of a system where the atom count is changing due to evaporation, you typically should use the *compute_modify dynamic yes* command for the temperature compute you are using.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix computes a global scalar, which can be accessed by various *output commands*. The scalar is the cumulative number of deleted atoms. The scalar value calculated by this fix is "intensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.48.4 Restrictions

This fix is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.48.5 Related commands

fix deposit

16.48.6 Default

The option defaults are molecule = no.

16.49 fix external command

16.49.1 Syntax

```
fix ID group-ID external mode args
```

- ID, group-ID are documented in *fix* command
- external = style name of this fix command
- mode = *pf/callback* or *pf/array*

```
pf/callback args = Ncall Napply
  Ncall = make callback every Ncall steps
  Napply = apply callback forces every Napply steps
pf/array args = Napply
  Napply = apply array forces every Napply steps
```

16.49.2 Examples

```
fix 1 all external pf/callback 1 1
fix 1 all external pf/callback 100 1
fix 1 all external pf/array 10
```

16.49.3 Description

This fix allows external programs that are running LAMMPS through its *library interface* to modify certain LAMMPS properties on specific timesteps, similar to the way other fixes do. The external driver can be a *C/C++ or Fortran program* or a *Python script*.

If mode is *pf/callback* then the fix will make a callback every *Ncall* timesteps or minimization iterations to the external program. The external program computes forces on atoms by setting values in an array owned by the fix. The fix then adds these forces to each atom in the group, once every *Napply* steps, similar to the way the *fix addforce* command works. Note that if *Ncall* > *Napply*, the force values produced by one callback will persist, and be used multiple times to update atom forces.

The callback function "foo" is invoked by the fix as:

```
foo(void *ptr, bigint timestep, int nlocal, int *ids, double **x, double
↪**fexternal);
```

The arguments are as follows:

- ptr = pointer provided by and simply passed back to external driver
- timestep = current LAMMPS timestep
- nlocal = # of atoms on this processor

- ids = list of atom IDs on this processor
- x = coordinates of atoms on this processor
- fexternal = forces to add to atoms on this processor

Note that timestep is a "bigint" which is defined in src/lmptype.h, typically as a 64-bit integer.

Fexternal are the forces returned by the driver program.

The fix has a set_callback() method which the external driver can call to pass a pointer to its foo() function. See the couple/lammps_quest/lmpqst.cpp file in the LAMMPS distribution for an example of how this is done. This sample application performs classical MD using quantum forces computed by a density functional code Quest.

If mode is *pf/array* then the fix simply stores force values in an array. The fix adds these forces to each atom in the group, once every *Napply* steps, similar to the way the *fix addforce* command works.

The name of the public force array provided by the FixExternal class is

```
double **fexternal;
```

It is allocated by the FixExternal class as an (N,3) array where N is the number of atoms owned by a processor. The 3 corresponds to the fx, fy, fz components of force.

It is up to the external program to set the values in this array to the desired quantities, as often as desired. For example, the driver program might perform an MD run in stages of 1000 timesteps each. In between calls to the LAMMPS *run* command, it could retrieve atom coordinates from LAMMPS, compute forces, set values in fexternal, etc.

To use this fix during energy minimization, the energy corresponding to the added forces must also be set so as to be consistent with the added forces. Otherwise the minimization will not converge correctly.

This can be done from the external driver by calling this public method of the FixExternal class:

```
void set_energy(double eng);
```

where eng is the potential energy. Eng is an extensive quantity, meaning it should be the sum over per-atom energies of all affected atoms. It should also be provided in *energy units* consistent with the simulation. See the details below for how to insure this energy setting is used appropriately in a minimization.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify* *energy* option is supported by this fix to add the potential "energy" set by the external driver to the system's potential energy as part of *thermodynamic output*. This is a fictitious quantity but is needed so that the *minimize* command can include the forces added by this fix in a consistent manner. I.e. there is a decrease in potential energy when atoms move in the direction of the added force.

The *fix_modify* *virial* option is supported by this fix to add the contribution due to the interactions computed by the external program to the system's virial as part of *thermodynamic output*. The default is *virial yes*

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the potential energy discussed above. The scalar stored by this fix is "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command.

Note: If you want the fictitious potential energy associated with the added forces to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the *fix_modify energy* option for this fix.

16.49.4 Restrictions

none

Related commands: none

Default: none

16.50 fix ffl command

16.50.1 Syntax

```
fix ID id-group ffl tau Tstart Tstop seed [flip-type]
```

- ID, group-ID are documented in *fix* command
- ffl = style name of this fix command
- tau = thermostat parameter (positive real)
- Tstart, Tstop = temperature ramp during the run
- seed = random number seed to use for generating noise (positive integer)
- one more value may be appended

```
flip-type  = determines the flipping type, can be chosen between rescale - no_
↪flip - hard - soft, if no flip type is given, rescale will be chosen by default
```

16.50.2 Examples

```
fix 3 boundary ffl 10 300 300 31415
fix 1 all ffl 100 500 500 9265 soft
```

16.50.3 Description

Apply a Fast-Forward Langevin Equation (FFL) thermostat as described in *(Hijazi)*. Contrary to *fix langevin*, this fix performs both thermostatting and evolution of the Hamiltonian equations of motion, so it should not be used together with *fix nve* – at least not on the same atom groups.

The time-evolution of a single particle undergoing Langevin dynamics is described by the equations

$$\frac{dq}{dt} = \frac{p}{m},$$

$$\frac{dp}{dt} = -\gamma p + W + F,$$

where F is the physical force, γ is the friction coefficient, and W is a Gaussian random force.

The friction coefficient is the inverse of the thermostat parameter : $\gamma = 1/\tau$, with τ the thermostat parameter *tau*. The thermostat parameter is given in the time units, γ is in inverse time units.

Equilibrium sampling a temperature T is obtained by specifying the target value as the *Tstart* and *Tstop* arguments, so that the internal constants depending on the temperature are computed automatically.

The random number *seed* must be a positive integer. A Marsaglia random number generator is used. Each processor uses the input seed to generate its own unique seed and its own stream of random numbers. Thus the dynamics of the system will not be identical on two runs on different numbers of processors.

The flipping type *flip-type* can be chosen between 4 types described in *(Hijazi)*. The flipping operation occurs during the thermostatting step and it flips the momenta of the atoms. If no_flip is chosen, no flip will be executed and the integration will be the same as a standard Langevin thermostat *(Bussi)*. The other flipping types are : rescale - hard - soft.

Restart, fix_modify, output, run start/stop, minimize info:

The instantaneous values of the extended variables are written to *binary restart files*. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior. Note however that you should use a different seed each time you restart, otherwise the same sequence of random numbers will be used each time, which might lead to stochastic synchronization and subtle artifacts in the sampling.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

The *fix_modify energy* option is supported by this fix to add the energy change induced by Langevin thermostatting to the system's potential energy as part of *thermodynamic output*.

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the cumulative energy change due to this fix. The scalar value calculated by this fix is "extensive".

16.50.4 Restrictions

In order to perform constant-pressure simulations please use *fix press/berendsen*, rather than *fix npt*, to avoid duplicate integration of the equations of motion.

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.50.5 Related commands

fix nvt, *fix temp/rescale*, *fix viscous*, *fix nvt*, *pair_style dpd/tstat*, *fix gld*, *fix gle*

(Hijazi) M. Hijazi, D. M. Wilkins, M. Ceriotti, J. Chem. Phys. 148, 184109 (2018)

(Bussi) G. Bussi, M. Parrinello, Phs. Rev. E 75, 056707 (2007)

16.51 fix filter/corotate command

16.51.1 Syntax

```
fix ID group-ID filter/corotate keyword value ...
```

- ID, group-ID are documented in *fix* command
- one or more constraint/value pairs are appended
- constraint = *b* or *a* or *t* or *m*

```
b values = one or more bond types
a values = one or more angle types
t values = one or more atom types
m value = one or more mass values
```

16.51.2 Examples

```
timestep 8
run_style respa 3 2 8 bond 1 pair 2 kspace 3
fix cor all filter/corotate m 1.0

fix cor all filter/corotate b 4 19 a 3 5 2
```

16.51.3 Description

This fix implements a corotational filter for a mollified impulse method. In biomolecular simulations, it allows the usage of larger timesteps for long-range electrostatic interactions. For details, see *(Fath)*.

When using *run_style respa* for a biomolecular simulation with high-frequency covalent bonds, the outer time-step is restricted to below ~ 4fs due to resonance problems. This fix filters the outer stage of the respa and thus a larger (outer) time-step can be used. Since in large biomolecular simulations the computation of the long-range electrostatic contributions poses a major bottleneck, this can significantly accelerate the simulation.

The filter computes a cluster decomposition of the molecular structure following the criteria indicated by the options a, b, t and m. This process is similar to the approach in *fix shake*, however, the clusters are not kept constrained. Instead, the position is slightly modified only for the computation of long-range forces. A good cluster decomposition constitutes in building clusters which contain the fastest covalent bonds inside clusters.

If the clusters are chosen suitably, the *run_style respa* is stable for outer time-steps of at least 8fs.

Restart, fix_modify, output, run start/stop, minimize info:

No information about these fixes is written to *binary restart files*. None of the *fix_modify* options are relevant to these fixes. No global or per-atom quantities are stored by these fixes for access by various *output commands*. No parameter of these fixes can be used with the *start/stop* keywords of the *run* command. These fixes are not invoked during *energy minimization*.

16.51.4 Restrictions

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Currently, it does not support *molecule templates*.

16.51.5 Related commands

Default: none

(Fath) Fath, Hochbruck, Singh, J Comp Phys, 333, 180-198 (2017).

16.52 fix flow/gauss command

16.52.1 Syntax

```
fix ID group-ID flow/gauss xflag yflag zflag keyword
```

- ID, group-ID are documented in *fix* command
- flow/gauss = style name of this fix command
- xflag,yflag,zflag = 0 or 1

```
0 = do not conserve current in this dimension
1 = conserve current in this dimension
```

- zero or more keyword/value pairs may be appended
- keyword = *energy*

```
energy value = no or yes
  no = do not compute work done by this fix
  yes = compute work done by this fix
```

16.52.2 Examples

```
fix GD fluid flow/gauss 1 0 0
fix GD fluid flow/gauss 1 1 1 energy yes
```

16.52.3 Description

This fix implements the Gaussian dynamics (GD) method to simulate a system at constant mass flux *(Strong)*. GD is a nonequilibrium molecular dynamics simulation method that can be used to study fluid flows through pores, pipes, and channels. In its original implementation GD was used to compute the pressure required to achieve a fixed mass flux through an opening. The flux can be conserved in any combination of the directions, x, y, or z, using xflag,yflag,zflag. This fix does not initialize a net flux through a system, it only conserves the center-of-mass momentum that is present when the fix is declared in the input script. Use the *velocity* command to generate an initial center-of-mass momentum.

GD applies an external fluctuating gravitational field that acts as a driving force to keep the system away from equilibrium. To maintain steady state, a profile-unbiased thermostat must be implemented to dissipate the heat that is added by the driving force. *Compute temp/profile* can be used to implement a profile-unbiased thermostat.

A common use of this fix is to compute a pressure drop across a pipe, pore, or membrane. The pressure profile can be computed in LAMMPS with *compute stress/atom* and *fix ave/chunk*, or with the hardy method in *fix atc*. Note that the simple *compute stress/atom* method is only accurate away from inhomogeneities in the fluid, such as fixed wall atoms. Further, the computed pressure profile must be corrected for the acceleration applied by GD before computing a pressure drop or comparing it to other methods, such as the pump method *(Zhu)*. The pressure correction is discussed and described in *(Strong)*.

For a complete example including the considerations discussed above, see the examples/USER/flow_gauss directory.

Note: Only the flux of the atoms in group-ID will be conserved. If the velocities of the group-ID atoms are coupled to the velocities of other atoms in the simulation, the flux will not be conserved. For example, in a simulation with fluid atoms and harmonically constrained wall atoms, if a single thermostat is applied to group *all*, the fluid atom velocities will be coupled to the wall atom velocities, and the flux will not be conserved. This issue can be avoided by thermostatting the fluid and wall groups separately.

Adding an acceleration to atoms does work on the system. This added energy can be optionally subtracted from the potential energy for the thermodynamic output (see below) to check that the timestep is small enough to conserve energy. Since the applied acceleration is fluctuating in time, the work cannot be computed from a potential. As a result, computing the work is slightly more computationally expensive than usual, so it is not performed by default. To invoke the work calculation, use the *energy* keyword. The *fix_modify energy* option also invokes the work calculation, and overrides an *energy no* setting here. If neither *energy yes* or *fix_modify energy yes* are set, the global scalar computed by the fix will return zero.

Note: In order to check energy conservation, any other fixes that do work on the system must have *fix_modify energy yes* set as well. This includes thermostat fixes and any constraints that hold the positions of wall atoms fixed, such as *fix spring/self*.

If this fix is used in a simulation with the *rRESPA* integrator, the applied acceleration must be computed and applied at the same rRESPA level as the interactions between the flowing fluid and the obstacle. The rRESPA level at which the acceleration is applied can be changed using the *fix_modify respa* option discussed below. If the flowing fluid and the obstacle interact through multiple interactions that are computed at different rRESPA levels, then there must be a separate flow/gauss fix for each level. For example, if the flowing fluid and obstacle interact through pairwise and long-range Coulomb interactions, which are computed at rRESPA levels 3 and 4, respectively, then there must be two separate flow/gauss fixes, one that specifies *fix_modify respa 3* and one with *fix_modify respa 4*.

Restart, fix_modify, output, run start/stop, minimize info:

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

No information about this fix is written to *binary restart files*.

The *fix_modify energy* option is supported by this fix to subtract the work done from the system's potential energy as part of *thermodynamic output*.

The *fix_modify respa* option is supported by this fix. This allows the user to set at which level of the *rRESPA* integrator the fix computes and adds the external acceleration. Default is the outermost level.

This fix computes a global scalar and a global 3-vector of forces, which can be accessed by various *output commands*. The scalar is the negative of the work done on the system, see above discussion. The vector is the total force that

this fix applied to the group of atoms on the current timestep. The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

16.52.4 Restrictions

none

16.52.5 Related commands

fix addforce, *compute temp/profile*, *velocity*

16.52.6 Default

The option default for the *energy* keyword is energy = no.

(Strong) Strong and Eaves, J. Phys. Chem. B 121, 189 (2017).

(Evans) Evans and Morriss, Phys. Rev. Lett. 56, 2172 (1986).

(Zhu) Zhu, Tajkhorshid, and Schulten, Biophys. J. 83, 154 (2002).

16.53 fix freeze command

16.54 fix freeze/kk command

16.54.1 Syntax

```
fix ID group-ID freeze
```

- ID, group-ID are documented in *fix* command
- freeze = style name of this fix command

16.54.2 Examples

```
fix 2 bottom freeze
```

16.54.3 Description

Zero out the force and torque on a granular particle. This is useful for preventing certain particles from moving in a simulation. The *granular pair styles* also detect if this fix has been defined and compute interactions between frozen and non-frozen particles appropriately, as if the frozen particle has infinite mass. A similar functionality for normal (point) particles can be obtained using *fix setforce*.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix computes a global 3-vector of forces, which can be accessed by various *output commands*. This is the total force on the group of atoms before the forces on individual atoms are changed by the fix. The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.54.4 Restrictions

This fix is part of the GRANULAR package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

There can only be a single freeze fix defined. This is because other the *granular pair styles* treat frozen particles differently and need to be able to reference a single group to which this fix is applied.

16.54.5 Related commands

atom_style sphere, *fix setforce*

Default: none

16.55 fix gcmc command

16.55.1 Syntax

```
fix ID group-ID gcmc N X M type seed T mu displace keyword values ...
```

- ID, group-ID are documented in *fix* command
- gcmc = style name of this fix command
- N = invoke this fix every N steps
- X = average number of GCMC exchanges to attempt every N steps
- M = average number of MC moves to attempt every N steps
- type = atom type for inserted atoms (must be 0 if mol keyword used)
- seed = random # seed (positive integer)
- T = temperature of the ideal gas reservoir (temperature units)
- mu = chemical potential of the ideal gas reservoir (energy units)
- displace = maximum Monte Carlo translation distance (length units)
- zero or more keyword/value pairs may be appended to args

```
keyword = mol, region, maxangle, pressure, fugacity_coeff, full_energy,␣
↪charge, group, grouptype, intra_energy, tfac_insert, or overlap_cutoff
  mol value = template-ID
    template-ID = ID of molecule template specified in a separate␣
↪molecule command
  mcmoves values = Patomtrans Pmoltrans Pmolrotate
    Patomtrans = proportion of atom translation MC moves
    Pmoltrans = proportion of molecule translation MC moves
    Pmolrotate = proportion of molecule rotation MC moves
  rigid value = fix-ID
    fix-ID = ID of fix rigid/small command
  shake value = fix-ID
    fix-ID = ID of fix shake command
  region value = region-ID
    region-ID = ID of region where GCMC exchanges and MC moves are allowed
  maxangle value = maximum molecular rotation angle (degrees)
  pressure value = pressure of the gas reservoir (pressure units)
  fugacity_coeff value = fugacity coefficient of the gas reservoir␣
↪(unitless)
  full_energy = compute the entire system energy when performing GCMC␣
↪exchanges and MC moves
  charge value = charge of inserted atoms (charge units)
  group value = group-ID
    group-ID = group-ID for inserted atoms (string)
  grouptype values = type group-ID
    type = atom type (int)
    group-ID = group-ID for inserted atoms (string)
  intra_energy value = intramolecular energy (energy units)
  tfac_insert value = scale up/down temperature of inserted atoms␣
↪(unitless)
```

```
  overlap_cutoff value = maximum pair distance for overlap rejection␣
↪(distance units)
  max value = Maximum number of molecules allowed in the system
  min value = Minimum number of molecules allowed in the system
```

16.55.2 Examples

```
fix 2 gas gcmc 10 1000 1000 2 29494 298.0 -0.5 0.01
fix 3 water gcmc 10 100 100 0 3456543 3.0 -2.5 0.1 mol my_one_water maxangle 180 full_
↪energy
fix 4 my_gas gcmc 1 10 10 1 123456543 300.0 -12.5 1.0 region disk
```

16.55.3 Description

This fix performs grand canonical Monte Carlo (GCMC) exchanges of atoms or molecules with an imaginary ideal gas reservoir at the specified T and chemical potential (mu) as discussed in *(Frenkel)*. It also attempts Monte Carlo (MC) moves (translations and molecule rotations) within the simulation cell or region. If used with the *fix nvt* command, simulations in the grand canonical ensemble (muVT, constant chemical potential, constant volume, and constant temperature) can be performed. Specific uses include computing isotherms in microporous materials, or computing vapor-liquid coexistence curves.

Every N timesteps the fix attempts both GCMC exchanges (insertions or deletions) and MC moves of gas atoms or molecules. On those timesteps, the average number of attempted GCMC exchanges is X, while the average number of attempted MC moves is M. For GCMC exchanges of either molecular or atomic gasses, these exchanges can be either deletions or insertions, with equal probability.

The possible choices for MC moves are translation of an atom, translation of a molecule, and rotation of a molecule. The relative amounts of each are determined by the optional *mcmoves* keyword (see below). The default behavior is as follows. If the *mol* keyword is used, only molecule translations and molecule rotations are performed with equal probability. Conversely, if the *mol* keyword is not used, only atom translations are performed. M should typically be chosen to be approximately equal to the expected number of gas atoms or molecules of the given type within the simulation cell or region, which will result in roughly one MC move per atom or molecule per MC cycle.

All inserted particles are always added to two groups: the default group "all" and the fix group specified in the fix command. In addition, particles are also added to any groups specified by the *group* and *grouptype* keywords. If inserted particles are individual atoms, they are assigned the atom type given by the type argument. If they are molecules, the type argument has no effect and must be set to zero. Instead, the type of each atom in the inserted molecule is specified in the file read by the *molecule* command.

Note: Care should be taken to apply fix gcmc only to a group that contains only those atoms and molecules that you wish to manipulate using Monte Carlo. Hence it is generally not a good idea to specify the default group "all" in the fix command, although it is allowed.

This fix cannot be used to perform GCMC insertions of gas atoms or molecules other than the exchanged type, but GCMC deletions, and MC translations, and rotations can be performed on any atom/molecule in the fix group. All atoms in the simulation cell can be moved using regular time integration translations, e.g. via *fix nvt*, resulting in a hybrid GCMC+MD simulation. A smaller-than-usual timestep size may be needed when running such a hybrid simulation, especially if the inserted molecules are not well equilibrated.

This command may optionally use the *region* keyword to define an exchange and move volume. The specified region must have been previously defined with a *region* command. It must be defined with side = *in*. Insertion attempts occur only within the specified region. For non-rectangular regions, random trial points are generated within the rectangular bounding box until a point is found that lies inside the region. If no valid point is generated after 1000

trials, no insertion is performed, but it is counted as an attempted insertion. Move and deletion attempt candidates are selected from gas atoms or molecules within the region. If there are no candidates, no move or deletion is performed, but it is counted as an attempt move or deletion. If an attempted move places the atom or molecule center-of-mass outside the specified region, a new attempted move is generated. This process is repeated until the atom or molecule center-of-mass is inside the specified region.

If used with *fix nvt*, the temperature of the imaginary reservoir, T, should be set to be equivalent to the target temperature used in fix nvt. Otherwise, the imaginary reservoir will not be in thermal equilibrium with the simulation cell. Also, it is important that the temperature used by fix nvt be dynamic/dof, which can be achieved as follows:

```
compute mdtemp mdatoms temp
compute_modify mdtemp dynamic/dof yes
fix mdnvt mdatoms nvt temp 300.0 300.0 10.0
fix_modify mdnvt temp mdtemp
```

Note that neighbor lists are re-built every timestep that this fix is invoked, so you should not set N to be too small. However, periodic rebuilds are necessary in order to avoid dangerous rebuilds and missed interactions. Specifically, avoid performing so many MC translations per timestep that atoms can move beyond the neighbor list skin distance. See the *neighbor* command for details.

When an atom or molecule is to be inserted, its coordinates are chosen at a random position within the current simulation cell or region, and new atom velocities are randomly chosen from the specified temperature distribution given by T. The effective temperature for new atom velocities can be increased or decreased using the optional keyword *tfac_insert* (see below). Relative coordinates for atoms in a molecule are taken from the template molecule provided by the user. The center of mass of the molecule is placed at the insertion point. The orientation of the molecule is chosen at random by rotating about this point.

Individual atoms are inserted, unless the *mol* keyword is used. It specifies a *template-ID* previously defined using the *molecule* command, which reads a file that defines the molecule. The coordinates, atom types, charges, etc., as well as any bonding and special neighbor information for the molecule can be specified in the molecule file. See the *molecule* command for details. The only settings required to be in this file are the coordinates and types of atoms in the molecule.

When not using the *mol* keyword, you should ensure you do not delete atoms that are bonded to other atoms, or LAMMPS will soon generate an error when it tries to find bonded neighbors. LAMMPS will warn you if any of the atoms eligible for deletion have a non-zero molecule ID, but does not check for this at the time of deletion.

If you wish to insert molecules using the *mol* keyword that will be treated as rigid bodies, use the *rigid* keyword, specifying as its value the ID of a separate *fix rigid/small* command which also appears in your input script.

Note: If you wish the new rigid molecules (and other rigid molecules) to be thermostatted correctly via *fix rigid/small/nvt* or *fix rigid/small/npt*, then you need to use the "fix_modify dynamic/dof yes" command for the rigid fix. This is to inform that fix that the molecule count will vary dynamically.

If you wish to insert molecules via the *mol* keyword, that will have their bonds or angles constrained via SHAKE, use the *shake* keyword, specifying as its value the ID of a separate *fix shake* command which also appears in your input script.

Optionally, users may specify the relative amounts of different MC moves using the *mcmoves* keyword. The values *Patomtrans*, *Pmoltrans*, *Pmolrotate* specify the average proportion of atom translations, molecule translations, and molecule rotations, respectively. The values must be non-negative integers or real numbers, with at least one non-zero value. For example, (10,30,0) would result in 25% of the MC moves being atomic translations, 75% molecular translations, and no molecular rotations.

Optionally, users may specify the maximum rotation angle for molecular rotations using the *maxangle* keyword and specifying the angle in degrees. Rotations are performed by generating a random point on the unit sphere and a random rotation angle on the range [0,maxangle). The molecule is then rotated by that angle about an axis passing through

the molecule center of mass. The axis is parallel to the unit vector defined by the point on the unit sphere. The same procedure is used for randomly rotating molecules when they are inserted, except that the maximum angle is 360 degrees.

Note that fix gcmc does not use configurational bias MC or any other kind of sampling of intramolecular degrees of freedom. Inserted molecules can have different orientations, but they will all have the same intramolecular configuration, which was specified in the molecule command input.

For atomic gasses, inserted atoms have the specified atom type, but deleted atoms are any atoms that have been inserted or that already belong to the fix group. For molecular gasses, exchanged molecules use the same atom types as in the template molecule supplied by the user. In both cases, exchanged atoms/molecules are assigned to two groups: the default group "all" and the fix group (which can also be "all").

The chemical potential is a user-specified input parameter defined as:

$$\mu = \mu^{id} + \mu^{ex}$$

The second term mu_ex is the excess chemical potential due to energetic interactions and is formally zero for the fictitious gas reservoir but is non-zero for interacting systems. So, while the chemical potential of the reservoir and the simulation cell are equal, mu_ex is not, and as a result, the densities of the two are generally quite different. The first term mu_id is the ideal gas contribution to the chemical potential. mu_id can be related to the density or pressure of the fictitious gas reservoir by:

$$\begin{aligned}\mu^{id} =& kT \ln \rho \Lambda^3 \\ =& kT \ln \frac{\phi P \Lambda^3}{kT}\end{aligned}$$

where *k* is Boltzman's constant, *T* is the user-specified temperature, ρ is the number density, *P* is the pressure, and ϕ is the fugacity coefficient. The constant Λ is required for dimensional consistency. For all unit styles except *lj* it is defined as the thermal de Broglie wavelength

$$\Lambda = \sqrt{\frac{h^2}{2\pi m k T}}$$

where *h* is Planck's constant, and *m* is the mass of the exchanged atom or molecule. For unit style *lj*, Λ is simply set to unity. Note that prior to March 2017, Λ for unit style *lj* was calculated using the above formula with *h* set to the rather specific value of 0.18292026. Chemical potential under the old definition can be converted to an equivalent value under the new definition by subtracting $3kT \ln(\Lambda_{old})$.

As an alternative to specifying mu directly, the ideal gas reservoir can be defined by its pressure *P* using the *pressure* keyword, in which case the user-specified chemical potential is ignored. The user may also specify the fugacity coefficient ϕ using the *fugacity_coeff* keyword, which defaults to unity.

The *full_energy* option means that the fix calculates the total potential energy of the entire simulated system, instead of just the energy of the part that is changed. The total system energy before and after the proposed GCMC exchange or MC move is then used in the Metropolis criterion to determine whether or not to accept the proposed change. By default, this option is off, in which case only partial energies are computed to determine the energy difference due to the proposed change.

The *full_energy* option is needed for systems with complicated potential energy calculations, including the following:

- long-range electrostatics (kspace)
- many-body pair styles
- hybrid pair styles
- eam pair styles
- tail corrections

- need to include potential energy contributions from other fixes

In these cases, LAMMPS will automatically apply the *full_energy* keyword and issue a warning message.

When the *mol* keyword is used, the *full_energy* option also includes the intramolecular energy of inserted and deleted molecules, whereas this energy is not included when *full_energy* is not used. If this is not desired, the *intra_energy* keyword can be used to define an amount of energy that is subtracted from the final energy when a molecule is inserted, and subtracted from the initial energy when a molecule is deleted. For molecules that have a non-zero intramolecular energy, this will ensure roughly the same behavior whether or not the *full_energy* option is used.

Inserted atoms and molecules are assigned random velocities based on the specified temperature T. Because the relative velocity of all atoms in the molecule is zero, this may result in inserted molecules that are systematically too cold. In addition, the intramolecular potential energy of the inserted molecule may cause the kinetic energy of the molecule to quickly increase or decrease after insertion. The *tfac_insert* keyword allows the user to counteract these effects by changing the temperature used to assign velocities to inserted atoms and molecules by a constant factor. For a particular application, some experimentation may be required to find a value of *tfac_insert* that results in inserted molecules that equilibrate quickly to the correct temperature.

Some fixes have an associated potential energy. Examples of such fixes include: *efield*, *gravity*, *addforce*, *langevin*, *restrain*, *temp/berendsen*, *temp/rescale*, and *wall fixes*. For that energy to be included in the total potential energy of the system (the quantity used when performing GCMC exchange and MC moves), you MUST enable the *fix_modify energy* option for that fix. The doc pages for individual *fix* commands specify if this should be done.

Use the *charge* option to insert atoms with a user-specified point charge. Note that doing so will cause the system to become non-neutral. LAMMPS issues a warning when using long-range electrostatics (kspace) with non-neutral systems. See the *compute group/group* documentation for more details about simulating non-neutral systems with kspace on.

Use of this fix typically will cause the number of atoms to fluctuate, therefore, you will want to use the *compute_modify dynamic/dof* command to insure that the current number of atoms is used as a normalizing factor each time temperature is computed. A simple example of this is:

```
compute_modify thermo_temp dynamic yes
```

A more complicated example is listed earlier on this page in the context of NVT dynamics.

Note: If the density of the cell is initially very small or zero, and increases to a much larger density after a period of equilibration, then certain quantities that are only calculated once at the start (kspace parameters) may no longer be accurate. The solution is to start a new simulation after the equilibrium density has been reached.

With some pair_styles, such as *Buckingham*, *Born-Mayer-Huggins* and *ReaxFF*, two atoms placed close to each other may have an arbitrary large, negative potential energy due to the functional form of the potential. While these unphysical configurations are inaccessible to typical dynamical trajectories, they can be generated by Monte Carlo moves. The *overlap_cutoff* keyword suppresses these moves by effectively assigning an infinite positive energy to all new configurations that place any pair of atoms closer than the specified overlap cutoff distance.

The *max* and *min* keywords allow for the restriction of the number of atoms in the simulation. They automatically reject all insertion or deletion moves that would take the system beyond the set boundaries. Should the system already be beyond the boundary, only moves that bring the system closer to the bounds may be accepted.

The *group* keyword adds all inserted atoms to the *group* of the group-ID value. The *grouptype* keyword adds all inserted atoms of the specified type to the *group* of the group-ID value.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the fix to *binary restart files*. This includes information about the random number generator seed, the next timestep for MC exchanges, the number of MC step attempts and successes etc. See the *read_restart*

command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

Note: For this to work correctly, the timestep must **not** be changed after reading the restart with *reset_timestep*. The fix will try to detect it and stop with an error.

None of the *fix_modify* options are relevant to this fix.

This fix computes a global vector of length 8, which can be accessed by various *output commands*. The vector values are the following global cumulative quantities:

- 1 = translation attempts
- 2 = translation successes
- 3 = insertion attempts
- 4 = insertion successes
- 5 = deletion attempts
- 6 = deletion successes
- 7 = rotation attempts
- 8 = rotation successes

The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.55.4 Restrictions

This fix is part of the MC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Do not set "neigh_modify once yes" or else this fix will never be called. Reneighboring is required.

Can be run in parallel, but aspects of the GCMC part will not scale well in parallel. Only usable for 3D simulations.

When using fix gcmc in combination with fix shake or fix rigid, only GCMC exchange moves are supported, so the argument *M* must be zero.

Note that very lengthy simulations involving insertions/deletions of billions of gas molecules may run out of atom or molecule IDs and trigger an error, so it is better to run multiple shorter-duration simulations. Likewise, very large molecules have not been tested and may turn out to be problematic.

Use of multiple fix gcmc commands in the same input script can be problematic if using a template molecule. The issue is that the user-referenced template molecule in the second fix gcmc command may no longer exist since it might have been deleted by the first fix gcmc command. An existing template molecule will need to be referenced by the user for each subsequent fix gcmc command.

16.55.5 Related commands

fix atom/swap, *fix nvt*, *neighbor*, *fix deposit*, *fix evaporate*, *delete_atoms*

16.55.6 Default

The option defaults are mol = no, maxangle = 10, overlap_cutoff = 0.0, fugacity_coeff = 1.0, intra_energy = 0.0, tfac_insert = 1.0. (Patomtrans, Pmoltrans, Pmolrotate) = (1, 0, 0) for mol = no and (0, 1, 1) for mol = yes. full_energy = no, except for the situations where full_energy is required, as listed above.

(Frenkel) Frenkel and Smit, Understanding Molecular Simulation, Academic Press, London, 2002.

16.56 fix gld command

16.56.1 Syntax

```
fix ID group-ID gld Tstart Tstop N_k seed series c_1 tau_1 ... c_N_k tau_N_k keyword␣
↪values ...
```

- ID, group-ID are documented in *fix* command
- gld = style name of this fix command
- Tstart,Tstop = desired temperature at start/end of run (temperature units)
- N_k = number of terms in the Prony series representation of the memory kernel
- seed = random number seed to use for white noise (positive integer)
- series = *pprony* is presently the only available option
- c_k = the weight of the kth term in the Prony series (mass per time units)
- tau_k = the time constant of the kth term in the Prony series (time units)
- zero or more keyword/value pairs may be appended

```
keyword = frozen or zero
  frozen value = no or yes
    no = initialize extended variables using values drawn from␣
↪equilibrium distribution at Tstart
    yes = initialize extended variables to zero (i.e., from equilibrium␣
↪distribution at zero temperature)
  zero value = no or yes
    no = do not set total random force to zero
    yes = set total random force to zero
```

16.56.2 Examples

```
fix 1 all gld 1.0 1.0 2 82885 pprony 0.5 1.0 1.0 2.0 frozen yes zero yes
fix 3 rouse gld 7.355 7.355 4 48823 pprony 107.1 0.02415 186.0 0.04294 428.6 0.09661␣
↪1714 0.38643
```

16.56.3 Description

Applies Generalized Langevin Dynamics to a group of atoms, as described in *(Baczewski)*. This is intended to model the effect of an implicit solvent with a temporally non-local dissipative force and a colored Gaussian random force, consistent with the Fluctuation-Dissipation Theorem. The functional form of the memory kernel associated with the temporally non-local force is constrained to be a Prony series.

Note: While this fix bears many similarities to *fix langevin*, it has one significant difference. Namely, *fix gld* performs time integration, whereas *fix langevin* does NOT. To this end, the specification of another fix to perform time integration, such as *fix nve*, is NOT necessary.

With this fix active, the force on the *j*th atom is given as

$$\begin{aligned}
\mathbf{F}_j(t) =& \mathbf{F}_j^C(t) - \int_0^t \Gamma_j(t-s)\mathbf{v}_j(s)\,\mathrm{d}s + \mathbf{F}_j^R(t) \\
\Gamma_j(t-s) =& \sum_{k=1}^{N_k} \frac{c_k}{\tau_k} e^{-(t-s)/\tau_k} \\
\langle \mathbf{F}_j^R(t), \mathbf{F}_j^R(s) \rangle =& \mathrm{k_B T}\, \Gamma_j(t-s)
\end{aligned}$$

Here, the first term is representative of all conservative (pairwise, bonded, etc) forces external to this fix, the second is the temporally non-local dissipative force given as a Prony series, and the third is the colored Gaussian random force.

The Prony series form of the memory kernel is chosen to enable an extended variable formalism, with a number of exemplary mathematical features discussed in *(Baczewski)*. In particular, $3N_k$ extended variables are added to each atom, which effect the action of the memory kernel without having to explicitly evaluate the integral over time in the second term of the force. This also has the benefit of requiring the generation of uncorrelated random forces, rather than correlated random forces as specified in the third term of the force.

Presently, the Prony series coefficients are limited to being greater than or equal to zero, and the time constants are limited to being greater than zero. To this end, the value of series MUST be set to *pprony*, for now. Future updates will allow for negative coefficients and other representations of the memory kernel. It is with these updates in mind that the series option was included.

The units of the Prony series coefficients are chosen to be mass per time to ensure that the numerical integration scheme stably approaches the Newtonian and Langevin limits. Details of these limits, and the associated numerical concerns are discussed in *(Baczewski)*.

The desired temperature at each timestep is ramped from *Tstart* to *Tstop* over the course of the next run.

The random # *seed* must be a positive integer. A Marsaglia random number generator is used. Each processor uses the input seed to generate its own unique seed and its own stream of random numbers. Thus the dynamics of the system will not be identical on two runs on different numbers of processors.

The keyword/value option pairs are used in the following ways.

The keyword *frozen* can be used to specify how the extended variables associated with the GLD memory kernel are initialized. Specifying no (the default), the initial values are drawn at random from an equilibrium distribution at *Tstart*, consistent with the Fluctuation-Dissipation Theorem. Specifying yes, initializes the extended variables to zero.

The keyword *zero* can be used to eliminate drift due to the thermostat. Because the random forces on different atoms are independent, they do not sum exactly to zero. As a result, this fix applies a small random force to the entire system, and the center-of-mass of the system undergoes a slow random walk. If the keyword *zero* is set to *yes*, the total random force is set exactly to zero by subtracting off an equal part of it from each atom in the group. As a result, the center-of-mass of a system with zero initial momentum will not drift over time.

Restart, run start/stop, minimize info:

The instantaneous values of the extended variables are written to *binary restart files*. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior.

None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.56.4 Restrictions

This fix is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.56.5 Related commands

fix langevin, *fix viscous*, *pair_style dpd/tstat*

16.56.6 Default

The option defaults are frozen = no, zero = no.

(Baczewski) A.D. Baczewski and S.D. Bond, J. Chem. Phys. 139, 044107 (2013).

16.57 fix gle command

16.57.1 Syntax

```
fix ID id-group gle Ns Tstart Tstop seed Amatrix [noneq Cmatrix] [every stride]
```

- ID, group-ID are documented in *fix* command
- gle = style name of this fix command

- Ns = number of additional fictitious momenta
- Tstart, Tstop = temperature ramp during the run
- Amatrix = file to read the drift matrix A from
- seed = random number seed to use for generating noise (positive integer)
- zero or more keyword/value pairs may be appended

```
keyword = noneq or every
  noneq Cmatrix  = file to read the non-equilibrium covariance matrix␣
↪from
  every stride   = apply the GLE once every time steps. Reduces the␣
↪accuracy
      of the integration of the GLE, but has *no effect* on the accuracy␣
↪of equilibrium
      sampling. It might change sampling properties when used together␣
↪with noneq.
```

16.57.2 Examples

```
fix 3 boundary gle 6 300 300 31415 smart.A
fix 1 all gle 6 300 300 31415 qt-300k.A noneq qt-300k.C
```

16.57.3 Description

Apply a Generalized Langevin Equation (GLE) thermostat as described in *(Ceriotti)*. The formalism allows one to obtain a number of different effects ranging from efficient sampling of all vibrational modes in the system to inexpensive (approximate) modelling of nuclear quantum effects. Contrary to *fix langevin*, this fix performs both thermostatting and evolution of the Hamiltonian equations of motion, so it should not be used together with *fix nve* – at least not on the same atom groups.

Each degree of freedom in the thermostatted group is supplemented with Ns additional degrees of freedom s, and the equations of motion become

```
dq/dt=p/m
d(p,s)/dt=(F,0) - A(p,s) + B dW/dt
```

where F is the physical force, A is the drift matrix (that generalizes the friction in Langevin dynamics), B is the diffusion term and dW/dt un-correlated Gaussian random forces. The A matrix couples the physical (q,p) dynamics with that of the additional degrees of freedom, and makes it possible to obtain effectively a history-dependent noise and friction kernel.

The drift matrix should be given as an external file *Afile*, as a (Ns+1 x Ns+1) matrix in inverse time units. Matrices that are optimal for a given application and the system of choice can be obtained from *(GLE4MD)*.

Equilibrium sampling a temperature T is obtained by specifying the target value as the *Tstart* and *Tstop* arguments, so that the diffusion matrix that gives canonical sampling for a given A is computed automatically. However, the GLE framework also allow for non-equilibrium sampling, that can be used for instance to model inexpensively zero-point energy effects *(Ceriotti2)*. This is achieved specifying the *noneq* keyword followed by the name of the file that contains the static covariance matrix for the non-equilibrium dynamics. Please note, that the covariance matrix is expected to be given in **temperature units**.

Since integrating GLE dynamics can be costly when used together with simple potentials, one can use the *every* optional keyword to apply the Langevin terms only once every several MD steps, in a multiple time-step fashion. This

should be used with care when doing non-equilibrium sampling, but should have no effect on equilibrium averages when using canonical sampling.

The random number *seed* must be a positive integer. A Marsaglia random number generator is used. Each processor uses the input seed to generate its own unique seed and its own stream of random numbers. Thus the dynamics of the system will not be identical on two runs on different numbers of processors.

Note also that the Generalized Langevin Dynamics scheme that is implemented by the *fix gld* scheme is closely related to the present one. In fact, it should be always possible to cast the Prony series form of the memory kernel used by GLD into an appropriate input matrix for *fix gle*. While the GLE scheme is more general, the form used by *fix gld* can be more directly related to the representation of an implicit solvent environment.

Restart, fix_modify, output, run start/stop, minimize info:

The instantaneous values of the extended variables are written to *binary restart files*. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior. Note however that you should use a different seed each time you restart, otherwise the same sequence of random numbers will be used each time, which might lead to stochastic synchronization and subtle artifacts in the sampling.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

The *fix_modify energy* option is supported by this fix to add the energy change induced by Langevin thermostatting to the system's potential energy as part of *thermodynamic output*.

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the cumulative energy change due to this fix. The scalar value calculated by this fix is "extensive".

16.57.4 Restrictions

The GLE thermostat in its current implementation should not be used with rigid bodies, SHAKE or RATTLE. It is expected that all the thermostatted degrees of freedom are fully flexible, and the sampled ensemble will not be correct otherwise.

In order to perform constant-pressure simulations please use *fix press/berendsen*, rather than *fix npt*, to avoid duplicate integration of the equations of motion.

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.57.5 Related commands

fix nvt, *fix temp/rescale*, *fix viscous*, *fix nvt*, *pair_style dpd/tstat*, *fix gld*

(Ceriotti) Ceriotti, Bussi and Parrinello, J Chem Theory Comput 6, 1170-80 (2010)

(GLE4MD) http://gle4md.org/

(Ceriotti2) Ceriotti, Bussi and Parrinello, Phys Rev Lett 103, 030603 (2009)

16.58 fix gravity command

16.59 fix gravity/omp command

16.60 fix gravity/kk command

16.60.1 Syntax

```
fix ID group gravity magnitude style args
```

- ID, group are documented in *fix* command
- gravity = style name of this fix command
- magnitude = size of acceleration (force/mass units)
- magnitude can be a variable (see below)
- style = *chute* or *spherical* or *gradient* or *vector*

```
chute args = angle
  angle = angle in +x away from -z or -y axis in 3d/2d (in degrees)
  angle can be a variable (see below)
spherical args = phi theta
  phi = azimuthal angle from +x axis (in degrees)
  theta = angle from +z or +y axis in 3d/2d (in degrees)
  phi or theta can be a variable (see below)
vector args = x y z
  x y z = vector direction to apply the acceleration
  x or y or z can be a variable (see below)
```

16.60.2 Examples

```
fix 1 all gravity 1.0 chute 24.0
fix 1 all gravity v_increase chute 24.0
fix 1 all gravity 1.0 spherical 0.0 -180.0
fix 1 all gravity 10.0 spherical v_phi v_theta
fix 1 all gravity 100.0 vector 1 1 0
```

16.60.3 Description

Impose an additional acceleration on each particle in the group. This fix is typically used with granular systems to include a "gravity" term acting on the macroscopic particles. More generally, it can represent any kind of driving field, e.g. a pressure gradient inducing a Poiseuille flow in a fluid. Note that this fix operates differently than the *fix addforce* command. The addforce fix adds the same force to each atom, independent of its mass. This command imparts the same acceleration to each atom (force/mass).

The *magnitude* of the acceleration is specified in force/mass units. For granular systems (LJ units) this is typically 1.0. See the *units* command for details.

Style *chute* is typically used for simulations of chute flow where the specified *angle* is the chute angle, with flow occurring in the +x direction. For 3d systems, the tilt is away from the z axis; for 2d systems, the tilt is away from the y axis.

Style *spherical* allows an arbitrary 3d direction to be specified for the acceleration vector. *Phi* and *theta* are defined in the usual spherical coordinates. Thus for acceleration acting in the -z direction, *theta* would be 180.0 (or -180.0). *Theta* = 90.0 and *phi* = -90.0 would mean acceleration acts in the -y direction. For 2d systems, *phi* is ignored and *theta* is an angle in the xy plane where *theta* = 0.0 is the y-axis.

Style *vector* imposes an acceleration in the vector direction given by (x,y,z). Only the direction of the vector is important; it's length is ignored. For 2d systems, the *z* component is ignored.

Any of the quantities *magnitude*, *angle*, *phi*, *theta*, *x*, *y*, *z* which define the gravitational magnitude and direction, can be specified as an equal-style *variable*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the quantity. You should insure that the variable calculates a result in the appropriate units, e.g. force/mass or degrees.

Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent gravitational field.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify energy* option is supported by this fix to add the gravitational potential energy of the system to the system's potential energy as part of *thermodynamic output*.

The *fix_modify respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix is adding its forces. Default is the outermost level.

This fix computes a global scalar which can be accessed by various *output commands*. This scalar is the gravitational potential energy of the particles in the defined field, namely mass * (g dot x) for each particles, where x and mass are the particles position and mass, and g is the gravitational field. The scalar value calculated by this fix is "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.60.4 Restrictions

none

16.60.5 Related commands

atom_style sphere, *fix addforce*

Default: none

16.61 fix grem command

16.61.1 Syntax

```
fix ID group-ID grem lambda eta H0 thermostat-ID
```

- ID, group-ID are documented in *fix* command
- grem = style name of this fix command
- lambda = intercept parameter of linear effective temperature function
- eta = slope parameter of linear effective temperature function
- H0 = shift parameter of linear effective temperature function
- thermostat-ID = ID of Nose-Hoover thermostat or barostat used in simulation

16.61.2 Examples

```
fix             fxgREM all grem 400 -0.01 -30000 fxnpt
thermo_modify   press fxgREM_press

fix             fxgREM all grem 502 -0.15 -80000 fxnvt
```

16.61.3 Description

This fix implements the molecular dynamics version of the generalized replica exchange method (gREM) originally developed by *(Kim)*, which uses non-Boltzmann ensembles to sample over first order phase transitions. The is done by defining replicas with an enthalpy dependent effective temperature

$$T_{eff} = \lambda + \eta(H - H_0)$$

with η negative and steep enough to only intersect the characteristic microcanonical temperature (Ts) of the system once, ensuring a unimodal enthalpy distribution in that replica. λ is the intercept and effects the generalized ensemble similar to how temperature effects a Boltzmann ensemble. H_0 is a reference enthalpy, and is typically set as the lowest desired sampled enthalpy. Further explanation can be found in our recent papers *(Malolepsza)*.

This fix requires a Nose-Hoover thermostat fix reference passed to the grem as *thermostat-ID*. Two distinct temperatures exist in this generalized ensemble, the effective temperature defined above, and a kinetic temperature that controls the velocity distribution of particles as usual. Either constant volume or constant pressure algorithms can be used.

The fix enforces a generalized ensemble in a single replica only. Typically, this ideology is combined with replica exchange with replicas differing by λ only for simplicity, but this is not required. A multi-replica simulation can be run within the LAMMPS environment using the *temper/grem* command. This utilizes LAMMPS partition mode and requires the number of available processors be on the order of the number of desired replicas. A 100-replica simulation would require at least 100 processors (1 per world at minimum). If many replicas are needed on a small

number of processors, multi-replica runs can be run outside of LAMMPS. An example of this can be found in examples/USER/misc/grem and has no limit on the number of replicas per processor. However, this is very inefficient and error prone and should be avoided if possible.

In general, defining the generalized ensembles is unique for every system. When starting a many-replica simulation without any knowledge of the underlying microcanonical temperature, there are several tricks we have utilized to optimize the process. Choosing a less-steep η yields broader distributions, requiring fewer replicas to map the microcanonical temperature. While this likely struggles from the same sampling problems gREM was built to avoid, it provides quick insight to Ts. Initially using an evenly-spaced λ distribution identifies regions where small changes in enthalpy lead to large temperature changes. Replicas are easily added where needed.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *thermo_modify* *press* option is supported by this fix to add the rescaled kinetic pressure as part of *thermodynamic output*.

16.61.4 Restrictions

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.61.5 Related commands

temper/grem, *fix nvt*, *fix npt*, *thermo_modify*

Default: none

(Kim) Kim, Keyes, Straub, J Chem. Phys, 132, 224107 (2010).

(Malolepsza) Malolepsza, Secor, Keyes, J Phys Chem B 119 (42), 13379-13384 (2015).

16.62 fix halt command

16.62.1 Syntax

```
fix ID group-ID halt N attribute operator avalue keyword value ...
```

- ID, group-ID are documented in *fix* command
- halt = style name of this fix command
- N = check halt condition every N steps
- attribute = *bondmax* or *tlimit* or v_name

  ```
  bondmax = length of longest bond in the system
  tlimit = elapsed CPU time
  v_name = name of equal-style variable
  ```

- operator = "<" or "<=" or ">" or ">=" or "==" or "!=" or "|^"

- avalue = numeric value to compare attribute to
- zero or more keyword/value pairs may be appended
- keyword = *error* or *message*

  error value = *hard* or *soft* or *continue*
  message value = *yes* or *no*

16.62.2 Examples

```
fix 10 all halt 1 bondmax > 1.5
fix 10 all print 10 v_myCheck != 0 error soft
```

16.62.3 Description

Check a condition every N steps during a simulation run. N must be >= 1. If the condition is met, exit the run immediately. In this context a "run" can be dynamics or minimization iterations, as specified by the *run* or *minimize* command.

The specified group-ID is ignored by this fix.

The specified *attribute* can be one of the options listed above, namely *bondmax* or *tlimit*, or an *equal-style variable* referenced as *v_name*, where "name" is the name of a variable that has been defined previously in the input script.

The *bondmax* attribute will loop over all bonds in the system, compute their current lengths, and set *attribute* to the longest bond distance.

The *tlimit* attribute queries the elapsed CPU time (in seconds) since the current run began, and sets *attribute* to that value. This is an alternative way to limit the length of a simulation run, similar to the *timer* timeout command. There are two differences in using this method versus the timer command option. The first is that the clock starts at the beginning of the current run (not when the timer or fix command is specified), so that any setup time for the run is not included in the elapsed time. The second is that the timer invocation and syncing across all processors (via MPI_Allreduce) is not performed once every *N* steps by this command. Instead it is performed (typically) only a small number of times and the elapsed times are used to predict when the end-of-the-run will be. Both of these attributes can be useful when performing benchmark calculations for a desired length of time with minimal overhead. For example, if a run is performing 1000s of timesteps/sec, the overhead for syncing the timer frequently across a large number of processors may be non-negligible.

Equal-style variables evaluate to a numeric value. See the *variable* command for a description. They calculate formulas which can involve mathematical operations, atom properties, group properties, thermodynamic properties, global values calculated by a *compute* or *fix*, or references to other *variables*. Thus they are a very general means of computing some attribute of the current system. For example, the following "bondmax" variable will calculate the same quantity as the hstyle = bondmax option.

```
compute         bdist all bond/local dist
compute         bmax all reduce max c_bdist
variable        bondmax equal c_bmax
```

Thus these two versions of a fix halt command will do the same thing:

```
fix 10 all halt 1 bondmax > 1.5
fix 10 all halt 1 v_bondmax > 1.5
```

The version with "bondmax" will just run somewhat faster, due to less overhead in computing bond lengths and not storing them in a separate compute.

The choice of operators listed above are the usual comparison operators. The XOR operation (exclusive or) is also included as "|^". In this context, XOR means that if either the attribute or avalue is 0.0 and the other is non-zero, then the result is "true". Otherwise it is "false".

The specified *avalue* must be a numeric value.

The optional *error* keyword determines how the current run is halted. If its value is *hard*, then LAMMPS will stop with an error message.

If its value is *soft*, LAMMPS will exit the current run, but continue to execute subsequent commands in the input script. However, additional *run* or *minimize* commands will be skipped. For example, this allows a script to output the current state of the system, e.g. via a *write_dump* or *write_restart* command.

If its value is *continue*, the behavior is the same as for *soft*, except subsequent *run* or *minimize* commands are executed. This allows your script to remedy the condition that triggered the halt, if necessary. Note that you may wish use the *unfix* command on the fix halt ID, so that the same condition is not immediately triggered in a subsequent run.

The optional *message* keyword determines whether a message is printed to the screen and logfile when the halt condition is triggered. If *message* is set to yes, a one line message with the values that triggered the halt is printed. If *message* is set to no, no message is printed; the run simply exits. The latter may be desirable for post-processing tools that extract thermodynamic information from log files.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

16.62.4 Restrictions

none

16.62.5 Related commands

variable

16.62.6 Default

The option defaults are error = hard and message = yes.

16.63 fix heat command

16.63.1 Syntax

```
fix ID group-ID heat N eflux
```

- ID, group-ID are documented in *fix* command
- heat = style name of this fix command
- N = add/subtract heat every this many timesteps
- eflux = rate of heat addition or subtraction (energy/time units)

- eflux can be a variable (see below)
- zero or more keyword/value pairs may be appended to args
- keyword = *region*

```
region value = region-ID
  region-ID = ID of region atoms must be in to have added force
```

16.63.2 Examples

```
fix 3 qin heat 1 1.0
fix 3 qin heat 10 v_flux
fix 4 qout heat 1 -1.0 region top
```

16.63.3 Description

Add non-translational kinetic energy (heat) to a group of atoms in a manner that conserves their aggregate momentum. Two of these fixes can be used to establish a temperature gradient across a simulation domain by adding heat (energy) to one group of atoms (hot reservoir) and subtracting heat from another (cold reservoir). E.g. a simulation sampling from the McDLT ensemble.

If the *region* keyword is used, the atom must be in both the group and the specified geometric *region* in order to have energy added or subtracted to it. If not specified, then the atoms in the group are affected wherever they may move to.

Heat addition/subtraction is performed every N timesteps. The *eflux* parameter can be specified as a numeric constant or as a variable (see below). If it is a numeric constant or equal-style variable which evaluates to a scalar value, then the *eflux* determines the change in aggregate energy of the entire group of atoms per unit time, e.g. in eV/psec for *metal units*. In this case it is an "extensive" quantity, meaning its magnitude should be scaled with the number of atoms in the group. Note that since *eflux* has per-time units (i.e. it is a flux), this means that a larger value of N will add/subtract a larger amount of energy each time the fix is invoked.

Note: The heat-exchange (HEX) algorithm implemented by this fix is known to exhibit a pronounced energy drift. An improved algorithm (eHEX) is available as a *fix ehex* command and might be preferable if energy conservation is important.

If *eflux* is specified as an atom-style variable (see below), then the variable computes one value per atom. In this case, each value is the energy flux for a single atom, again in units of energy per unit time. In this case, each value is an "intensive" quantity, which need not be scaled with the number of atoms in the group.

As mentioned above, the *eflux* parameter can be specified as an equal-style or atom_style *variable*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value(s) used to determine the flux.

Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent flux.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent flux with optional time-dependence as well.

Note: If heat is subtracted from the system too aggressively so that the group's kinetic energy would go to zero, or any individual atom's kinetic energy would go to zero for the case where *eflux* is an atom-style variable, then LAMMPS

will halt with an error message.

Fix heat is different from a thermostat such as *fix nvt* or *fix temp/rescale* in that energy is added/subtracted continually. Thus if there isn't another mechanism in place to counterbalance this effect, the entire system will heat or cool continuously. You can use multiple heat fixes so that the net energy change is 0.0 or use *fix viscous* to drain energy from the system.

This fix does not change the coordinates of its atoms; it only scales their velocities. Thus you must still use an integration fix (e.g. *fix nve*) on the affected atoms. This fix should not normally be used on atoms that have their temperature controlled by another fix - e.g. *fix nvt* or *fix langevin* fix.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix computes a global scalar which can be accessed by various *output commands*. This scalar is the most recent value by which velocities were scaled. The scalar value calculated by this fix is "intensive". If *eflux* is specified as an atom-style variable, this fix computes the average value by which the velocities were scaled for all of the atoms that had their velocities scaled.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.63.4 Restrictions

none

16.63.5 Related commands

fix ehex, *compute temp*, *compute temp/region*

Default: none

16.64 fix hyper/global command

16.64.1 Syntax

```
fix ID group-ID hyper/global cutbond qfactor Vmax Tequil
```

- ID, group-ID are documented in *fix* command
- hyper/global = style name of this fix command
- cutbond = max distance at which a pair of atoms is considered bonded (distance units)
- qfactor = max strain at which bias potential goes to 0.0 (unitless)
- Vmax = height of bias potential (energy units)
- Tequil = equilibration temperature (temperature units)

16.64.2 Examples

```
fix 1 all hyper/global 1.0 0.3 0.8 300.0
```

16.64.3 Description

This fix is meant to be used with the *hyper* command to perform a bond-boost global hyperdynamics (GHD) simulation. The role of this fix is to a select a single pair of atoms in the system at each timestep to add a global bias potential to, which will alter the dynamics of the system in a manner that effectively accelerates time. This is in contrast to the *fix hyper/local* command, which can be user to perform a local hyperdynamics (LHD) simulation, by adding a local bias potential to multiple pairs of atoms at each timestep. GHD can time accelerate a small simulation with up to a few 100 atoms. For larger systems, LHD is needed to achieve good time acceleration.

For a system that undergoes rare transition events, where one or more atoms move over an energy barrier to a new potential energy basin, the effect of the bias potential is to induce more rapid transitions. This can lead to a dramatic speed-up in the rate at which events occurs, without altering their relative frequencies, thus leading to an overall increase in the elapsed real time of the simulation as compared to running for the same number of timesteps with normal MD. See the *hyper* doc page for a more general discussion of hyperdynamics and citations that explain both GHD and LHD.

The equations and logic used by this fix and described here to perform GHD follow the description given in *(Voter2013)*. The bond-boost form of a bias potential for HD is due to Miron and Fichthorn as described in *(Miron)*. In LAMMPS we use a simplified version of bond-boost GHD where a single bond in the system is biased at any one timestep.

Bonds are defined between each pair of atoms *ij*, whose R_{ij}^0 distance is less than *cutbond*, when the system is in a quenched state (minimum) energy. Note that these are not "bonds" in a covalent sense. A bond is simply any pair of atoms that meet the distance criterion. *Cutbond* is an argument to this fix; it is discussed below. A bond is only formed if one or both of the *ij* atoms are in the specified group.

The current strain of bond *ij* (when running dynamics) is defined as

$$E_{ij} = \frac{R_{ij} - R_{ij}^0}{R_{ij}^0}$$

where R_{ij} is the current distance between atoms *i* and *j*, and R_{ij}^0 is the equilibrium distance in the quenched state.

The bias energy V_{ij} of any bond between atoms *i* and *j* is defined as

$$V_{ij} = V^{max} \cdot \left(1 - \left(\frac{E_{ij}}{q}\right)^2\right) \text{ for } |E_{ij}| < qfactor \text{ or } 0 \text{ otherwise}$$

where the prefactor V^{max} and the cutoff *qfactor* are arguments to this fix; they are discussed below. This functional form is an inverse parabola centered at 0.0 with height V^{max} and which goes to 0.0 at +/- qfactor.

Let E^{max} be the maximum of $|E_{ij}|$ for all *ij* bonds in the system on a given timestep. On that step, V_{ij} is added as a bias potential to only the single bond with strain E^{max}, call it V_{ij}^{max}. Note that V_{ij}^{max} will be 0.0 if $E^{max} >=$ qfactor on that timestep. Also note that V_{ij}^{max} is added to the normal interatomic potential that is computed between all atoms in the system at every step.

The derivative of V_{ij}^{max} with respect to the position of each atom in the E^{max} bond gives a bias force F_{ij}^{max} acting on the bond as

$$F_{ij}^{max} = -\frac{dV_{ij}^{max}}{dE_{ij}} = \frac{2V^{max}E - ij}{\text{qfactor}^2} \text{ for } |E_{ij}| < \text{qfactor or } 0 \text{ otherwise}$$

which can be decomposed into an equal and opposite force acting on only the two *ij* atoms in the E^{max} bond.

The time boost factor for the system is given each timestep I by

$$B_i = e^{\beta V_{ij}^{max}}$$

where $\beta = \frac{1}{kT_{equil}}$, and T_{equil} is the temperature of the system and an argument to this fix. Note that $B_i >= 1$ at every step.

Note: To run a GHD simulation, the input script must also use the *fix langevin* command to thermostat the atoms at the same *Tequil* as specified by this fix, so that the system is running constant-temperature (NVT) dynamics. LAMMPS does not check that this is done.

The elapsed time t_{hyper} for a GHD simulation running for *N* timesteps is simply

$$t_{hyper} = \sum_{i=1,N} B - i \cdot dt$$

where *dt* is the timestep size defined by the *timestep* command. The effective time acceleration due to GHD is thus t_hyper / N*dt, where N*dt is elapsed time for a normal MD run of N timesteps.

Note that in GHD, the boost factor varies from timestep to timestep. Likewise, which bond has E^{max} strain and thus which pair of atoms the bias potential is added to, will also vary from timestep to timestep. This is in contrast to local hyperdynamics (LHD) where the boost factor is an input parameter; see the *fix hyper/local* doc page for details.

Here is additional information on the input parameters for GHD.

The *cutbond* argument is the cutoff distance for defining bonds between pairs of nearby atoms. A pair of *ij* atoms in their equilibrium, minimum-energy configuration, which are separated by a distance $R_{ij} < cutbond$, are flagged as a bonded pair. Setting *cubond* to be ~25% larger than the nearest-neighbor distance in a crystalline lattice is a typical choice for solids, so that bonds exist only between nearest neighbor pairs.

The *qfactor* argument is the limiting strain at which the bias potential goes to 0.0. It is dimensionless, so a value of 0.3 means a bond distance can be up to 30% larger or 30% smaller than the equilibrium (quenched) R0ij distance and the two atoms in the bond could still experience a non-zero bias force.

If *qfactor* is set too large, then transitions from one energy basin to another are affected because the bias potential is non-zero at the transition state (e.g. saddle point). If *qfactor* is set too small than little boost is achieved because the E_{ij} strain of some bond in the system will (nearly) always exceed *qfactor*. A value of 0.3 for *qfactor* is typically reasonable.

The *Vmax* argument is the prefactor on the bias potential. Ideally, tt should be set to a value slightly less than the smallest barrier height for an event to occur. Otherwise the applied bias potential may be large enough (when added to the interatomic potential) to produce a local energy basin with a maxima in the center. This can produce artificial energy minima in the same basin that trap an atom. Or if *Vmax* is even larger, it may induce an atom(s) to rapidly transition to another energy basin. Both cases are "bad dynamics" which violate the assumptions of GHD that guarantee an accelerated time-accurate trajectory of the system.

Note that if *Vmax* is set too small, the GHD simulation will run correctly. There will just be fewer events because the hyper time (t_hyper equation above) will be shorter.

Note: If you have no physical intuition as to the smallest barrier height in your system, a reasonable strategy to determine the largest *Vmax* you can use for a GHD model, is to run a sequence of simulations with smaller and smaller *Vmax* values, until the event rate does not change (as a function of hyper time).

The *Tequil* argument is the temperature at which the system is simulated; see the comment above about the *fix langevin* thermostatting. It is also part of the beta term in the exponential factor that determines how much boost is achieved as a function of the bias potential.

In general, the lower the value of *Tequil* and the higher the value of *Vmax*, the more time boost will be achievable by the GHD algorithm.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify* *energy* option is supported by this fix to add the energy of the bias potential to the system's potential energy as part of *thermodynamic output*.

This fix computes a global scalar and global vector of length 12, which can be accessed by various *output commands*. The scalar is the magnitude of the bias potential (energy units) applied on the current timestep. The vector stores the following quantities:

- 1 = boost factor on this step (unitless)
- 2 = max strain E_{ij} of any bond on this step (absolute value, unitless)
- 3 = ID of first atom in the max-strain bond
- 4 = ID of second atom in the max-strain bond
- 5 = average # of bonds/atom on this step
- 6 = fraction of timesteps where the biased bond has bias = 0.0 during this run
- 7 = fraction of timesteps where the biased bond has negative strain during this run
- 8 = max drift distance of any atom during this run (distance units)
- 9 = max bond length during this run (distance units)
- 10 = cumulative hyper time since fix was defined (time units)
- 11 = cumulative count of event timesteps since fix was defined
- 12 = cumulative count of atoms in events since fix was defined

The first 5 quantities are for the current timestep. Quantities 6-9 are for the current hyper run. They are reset each time a new hyper run is performed. Quantities 19-12 are cumulative across multiple runs (since the point in the input script the fix was defined).

For value 8, drift is the distance an atom moves between two quenched states when the second quench determines an event has occurred. Atoms involved in an event will typically move the greatest distance since others typically remain near their original quenched position.

For value 11, events are checked for by the *hyper* command once every *Nevent* timesteps. This value is the count of those timesteps on which one (or more) events was detected. It is NOT the number of distinct events, since more than one event may occur in the same *Nevent* time window.

For value 12, each time the *hyper* command checks for an event, it invokes a compute to flag zero or more atoms as participating in one or more events. E.g. atoms that have displaced more than some distance from the previous quench state. Value 11 is the cumulative count of the number of atoms participating in any of the events that were found.

The scalar and vector values calculated by this fix are all "intensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.64.4 Restrictions

This command can only be used if LAMMPS was built with the REPLICA package. See the *Build package* doc page for more info.

16.64.5 Related commands

hyper, *fix hyper/local*

Default: None

(Voter2013) S. Y. Kim, D. Perez, A. F. Voter, J Chem Phys, 139, 144110 (2013).

(Miron) R. A. Miron and K. A. Fichthorn, J Chem Phys, 119, 6210 (2003).

16.65 fix hyper/local command

16.65.1 Syntax

```
fix ID group-ID hyper/local cutbond qfactor Vmax Tequil Dcut alpha Btarget
```

- ID, group-ID are documented in *fix* command
- hyper/local = style name of this fix command
- cutbond = max distance at which a pair of atoms is considered bonded (distance units)
- qfactor = max strain at which bias potential goes to 0.0 (unitless)
- Vmax = estimated height of bias potential (energy units)
- Tequil = equilibration temperature (temperature units)
- Dcut = minimum distance between boosted bonds (distance units)
- alpha = boostostat relaxation time (time units)
- Btarget = desired time boost factor (unitless)
- zero or more keyword/value pairs may be appended
- keyword = *bound* or *reset* or *check/ghost* or *check/bias*

```
bound value = Bfrac
  Bfrac =  -1 or a value >= 0.0
reset value = Rfreq
  Rfreq = -1 or 0 or timestep value > 0
check/ghost values = none
check/bias values = Nevery error/warn/ignore
```

16.65.2 Examples

```
fix 1 all hyper/local 1.0 0.3 0.8 300.0
fix 1 all hyper/local 1.0 0.3 0.8 300.0 bound 0.1 reset 0
```

16.65.3 Description

This fix is meant to be used with the *hyper* command to perform a bond-boost local hyperdynamics (LHD) simulation. The role of this fix is to a select multiple pairs of atoms in the system at each timestep to add a local bias potential to, which will alter the dynamics of the system in a manner that effectively accelerates time. This is in contrast to the *fix hyper/global* command, which can be user to perform a global hyperdynamics (GHD) simulation, by adding a global bias potential to a single pair of atoms at each timestep. GHD can time accelerate a small simulation with up to a few 100 atoms. For larger systems, LHD is needed to achieve good time acceleration.

For a system that undergoes rare transition events, where one or more atoms move over an energy barrier to a new potential energy basin, the effect of the bias potential is to induce more rapid transitions. This can lead to a dramatic speed-up in the rate at which events occurs, without altering their relative frequencies, thus leading to an overall increase in the elapsed real time of the simulation as compared to running for the same number of timesteps with normal MD. See the *hyper* doc page for a more general discussion of hyperdynamics and citations that explain both GHD and LHD.

The equations and logic used by this fix and described here to perform LHD follow the description given in *(Voter2013)*. The bond-boost form of a bias potential for HD is due to Miron and Fichthorn as described in *(Miron)*.

To understand this description, you should first read the description of the GHD algorithm on the *fix hyper/global* doc page. This description of LHD builds on the GHD description.

The definition of bonds and E_{ij} are the same for GHD and LHD. The formulas for V_{ij}^{max} and F_{ij}^{max} are also the same except for a pre-factor C_{ij}, explained below.

The bias energy V_{ij} applied to a bond *ij* with maximum strain is

$$V_{ij}^{max} = C_{ij} \cdot V^{max} \cdot \left(1 - \left(\frac{E_{ij}}{q}\right)^2\right) \text{ for } |E_{ij}| < qfactor \text{ or } 0 \text{ otherwise}$$

The derivative of V_{ij}^{max} with respect to the position of each atom in the *ij* bond gives a bias force F_{ij}^{max} acting on the bond as

$$F_{ij}^{max} = -\frac{dV_{ij}^{max}}{dE_{ij}} = 2C_{ij}V^{max}\frac{E_{ij}}{qfactor^2} \text{ for } |E_{ij}| < qfactor \text{ or } 0 \text{ otherwise}$$

which can be decomposed into an equal and opposite force acting on only the two atoms *i* and *j* in the *ij* bond.

The key difference is that in GHD a bias energy and force is added (on a particular timestep) to only one bond (pair of atoms) in the system, which is the bond with maximum strain E^{max}.

In LHD, a bias energy and force can be added to multiple bonds separated by the specified *Dcut* distance or more. A bond *ij* is biased if it is the maximum strain bond within its local "neighborhood", which is defined as the bond *ij* plus any neighbor bonds within a distance *Dcut* from *ij*. The "distance" between bond *ij* and bond *kl* is the minimum distance between any of the *ik*, *il*, *jk*, and *jl* pairs of atoms.

For a large system, multiple bonds will typically meet this requirement, and thus a bias potential V_{ij}^{max} will be applied to many bonds on the same timestep.

In LHD, all bonds store a C_{ij} prefactor which appears in the V_{ij}^{max} and $F_{ij}^{max} equationsabove. Notethatthe : math :$ factor scales the strength of the bias energy and forces whenever bond *ij* is the maximum strain bond in its neighborhood.

C_{ij} is initialized to 1.0 when a bond between the *ij* atoms is first defined. The specified *Btarget* factor is then used to adjust the C_{ij} prefactors for each bond every timestep in the following manner.

An instantaneous boost factor B_{ij} is computed each timestep for each bond, as

$$B_{ij} = e^{\beta V_{kl}^{max}}$$

where V_{kl}^{max} is the bias energy of the maxstrain bond *kl* within bond *ij*'s neighborhood, $\beta = \frac{1}{kT_{equil}}$, and T_{equil} is the temperature of the system and an argument to this fix.

Note: To run an LHD simulation, the input script must also use the *fix langevin* command to thermostat the atoms at the same *Tequil* as specified by this fix, so that the system is running constant-temperature (NVT) dynamics. LAMMPS does not check that this is done.

Note that if *ij*== *kl*, then bond *ij* is a biased bond on that timestep, otherwise it is not. But regardless, the boost factor B_{ij} can be thought of an estimate of time boost currently being applied within a local region centered on bond *ij*. For LHD, we want this to be the specified *Btarget* value everywhere in the simulation domain.

To accomplish this, if $B_{ij} < B_{target}$, the C_{ij} prefactor for bond *ij* is incremented on the current timestep by an amount proportional to the inverse of the specified α and the difference $(B_{ij} - B_{target})$. Conversely if $B_{ij} > B_{target}$, C_{ij} is decremented by the same amount. This procedure is termed "boostostatting" in *(Voter2013)*. It drives all of the individual C_{ij} to values such that when V_{ij}^{max} is applied as a bias to bond *ij*, the resulting boost factor B_{ij} will be close to B_{target} on average. Thus the LHD time acceleration factor for the overall system is effectively *Btarget*.

Note that in LHD, the boost factor B_{target} is specified by the user. This is in contrast to global hyperdynamics (GHD) where the boost factor varies each timestep and is computed as a function of V_{max}, E_{max}, and T_{equil}; see the *fix hyper/global* doc page for details.

Here is additional information on the input parameters for LHD.

Note that the *cutbond*, *qfactor*, and *Tequil* arguments have the same meaning as for GHD. The *Vmax* argument is slightly different. The *Dcut*, *alpha*, and *Btarget* parameters are unique to LHD.

The *cutbond* argument is the cutoff distance for defining bonds between pairs of nearby atoms. A pair of I,J atoms in their equilibrium, minimum-energy configuration, which are separated by a distance $R_{ij} < cutbond$, are flagged as a bonded pair. Setting *cubond* to be ~25% larger than the nearest-neighbor distance in a crystalline lattice is a typical choice for solids, so that bonds exist only between nearest neighbor pairs.

The *qfactor* argument is the limiting strain at which the bias potential goes to 0.0. It is dimensionless, so a value of 0.3 means a bond distance can be up to 30% larger or 30% smaller than the equilibrium (quenched) R_{ij}^0 distance and the two atoms in the bond could still experience a non-zero bias force.

If *qfactor* is set too large, then transitions from one energy basin to another are affected because the bias potential is non-zero at the transition state (e.g. saddle point). If *qfactor* is set too small than little boost can be achieved because the E_{ij} strain of some bond in the system will (nearly) always exceed *qfactor*. A value of 0.3 for *qfactor* is typically a reasonable value.

The *Vmax* argument is a fixed prefactor on the bias potential. There is a also a dynamic prefactor C_{ij}, driven by the choice of *Btarget* as discussed above. The product of these should be a value less than the smallest barrier height for an event to occur. Otherwise the applied bias potential may be large enough (when added to the interatomic potential) to produce a local energy basin with a maxima in the center. This can produce artificial energy minima in the same basin that trap an atom. Or if $C_{ij} \cdot V^{max}$ is even larger, it may induce an atom(s) to rapidly transition to another energy basin. Both cases are "bad dynamics" which violate the assumptions of LHD that guarantee an accelerated time-accurate trajectory of the system.

Note: It may seem that V^{max} can be set to any value, and C_{ij} will compensate to reduce the overall prefactor if necessary. However the C_{ij} are initialized to 1.0 and the boostostatting procedure typically operates slowly enough that there can be a time period of bad dynamics if V^{max} is set too large. A better strategy is to set V^{max} to the slightly smaller than the lowest barrier height for an event (the same as for GHD), so that the C_{ij} remain near unity.

The *Tequil* argument is the temperature at which the system is simulated; see the comment above about the *fix langevin* thermostatting. It is also part of the beta term in the exponential factor that determines how much boost is achieved as a function of the bias potential. See the discussion of the *Btarget* argument below.

As discussed above, the *Dcut* argument is the distance required between two locally maxstrain bonds for them to both be selected as biased bonds on the same timestep. Computationally, the larger *Dcut* is, the more work (computation and communication) must be done each timestep within the LHD algorithm. And the fewer bonds can be simultaneously biased, which may mean the specified *Btarget* time acceleration cannot be achieved.

Physically *Dcut* should be a long enough distance that biasing two pairs of atoms that close together will not influence the dynamics of each pair. E.g. something like 2x the cutoff of the interatomic potential. In practice a *Dcut* value of ~10 Angstroms seems to work well for many solid-state systems.

Note: You should insure that ghost atom communication is performed for a distance of at least *Dcut* + *cutevent* = the distance one or more atoms move (between quenched states) to be considered an "event". It is an argument to the "compute event/displace" command used to detect events. By default the ghost communication distance is set by the pair_style cutoff, which will typically be < *Dcut*. The *comm_modify cutoff* command should be used to override the ghost cutoff explicitly, e.g.

```
comm_modify cutoff 12.0
```

Note that this fix does not know the *cutevent* parameter, but uses half the *cutbond* parameter as an estimate to warn if the ghost cutoff is not long enough.

As described above the *alpha* argument is a pre-factor in the boostostat update equation for each bond's C_{ij} prefactor. *Alpha* is specified in time units, similar to other thermostat or barostat damping parameters. It is roughly the physical time it will take the boostostat to adjust a C_{ij} value from a too high (or too low) value to a correct one. An *alpha* setting of a few ps is typically good for solid-state systems. Note that the *alpha* argument here is the inverse of the alpha parameter discussed in *(Voter2013)*.

The *Btarget* argument is the desired time boost factor (a value > 1) that all the atoms in the system will experience. The elapsed time t_hyper for an LHD simulation running for *N* timesteps is simply

$$t_{hyper} = B_{target} \cdot N \cdot dt$$

where *dt* is the timestep size defined by the *timestep* command. The effective time acceleration due to LHD is thus $\frac{t_{hyper}}{N \cdot dt} = B_{target}$, where $N \cdot dt$ is the elapsed time for a normal MD run of N timesteps.

You cannot choose an arbitrarily large setting for *Btarget*. The maximum value you should choose is

$$B_{target} = e^{\beta V_{small}}$$

where V_{small} is the smallest event barrier height in your system, $\beta = \frac{1}{kT_{equil}}$, and T_{equil} is the specified temperature of the system (both by this fix and the Langevin thermostat).

Note that if *Btarget* is set smaller than this, the LHD simulation will run correctly. There will just be fewer events because the hyper time (t_hyper equation above) will be shorter.

Note: If you have no physical intuition as to the smallest barrier height in your system, a reasonable strategy to

determine the largest *Btarget* you can use for an LHD model, is to run a sequence of simulations with smaller and smaller *Btarget* values, until the event rate does not change (as a function of hyper time).

Here is additional information on the optional keywords for this fix.

The *bound* keyword turns on min/max bounds for bias coefficients C_{ij} for all bonds. C_{ij} is a prefactor for each bond on the bias potential of maximum strength V^{max}. Depending on the choice of *alpha* and *Btarget* and *Vmax*, the boostostatting can cause individual C_{ij} values to fluctuate. If the fluctuations are too large $C_{ij} \cdot V^{max}$ can exceed low barrier heights and induce bad event dynamics. Bounding the C_{ij} values is a way to prevent this. If *Bfrac* is set to -1 or any negative value (the default) then no bounds are enforced on C_{ij} values (except they must always be >= 0.0). A *Bfrac* setting >= 0.0 sets a lower bound of 1.0 - Bfrac and upper bound of 1.0 + Bfrac on each C_{ij} value. Note that all C_{ij} values are initialized to 1.0 when a bond is created for the first time. Thus *Bfrac* limits the bias potential height to *Vmax* +/- *Bfrac*Vmax*.

The *reset* keyword allow *Vmax* to be adjusted dynamically depending on the average value of all C_{ij} prefactors. This can be useful if you are unsure what value of *Vmax* will match the *Btarget* boost for the system. The C_{ij} values will then adjust in aggregate (up or down) so that $C_{ij} \cdot V^{max}$ produces a boost of *Btarget*, but this may conflict with the *bound* keyword settings. By using *bound* and *reset* together, V^{max} itself can be reset, and desired bounds still applied to the C_{ij} values.

A setting for *Rfreq* of -1 (the default) means *Vmax* never changes. A setting of 0 means V^{max} is adjusted every time an event occurs and bond pairs are recalculated. A setting of N > 0 timesteps means V^{max} is adjusted on the first time an event occurs on a timestep >= N steps after the previous adjustment. The adjustment to V^{max} is computed as follows. The current average of all $C_{ij} \cdot V^{max}$ values is computed and the V^{max} is reset to that value. All C_{ij} values are changed to new prefactors such the new $C_{ij} \cdot V^{max}$ is the same as it was previously. If the *bound* keyword was used, those bounds are enforced on the new C_{ij} values. Henceforth, new bonds are assigned a $C_{ij} = 1.0$, which means their bias potential magnitude is the new V^{max}.

The *check/ghost* keyword turns on extra computation each timestep to compute statistics about ghost atoms used to determine which bonds to bias. The output of these stats are the vector values 14 and 15, described below. If this keyword is not enabled, the output of the stats will be zero.

The *check/bias* keyword turns on extra computation and communication to check if any biased bonds are closer than *Dcut* to each other, which should not be the case if LHD is operating correctly. Thus it is a debugging check. The *Nevery* setting determines how often the check is made. The *error*, *warn*, or *ignore* setting determines what is done if the count of too-close bonds is not zero. Either the code will exit, or issue a warning, or silently tally the count. The count can be output as vector value 17, as described below. If this keyword is not enabled, the output of that statistic will be 0.

Note that both of these computations are costly, hence they are only enabled by these keywords.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify energy* option is supported by this fix to add the energy of the bias potential to the system's potential energy as part of *thermodynamic output*.

This fix computes a global scalar and global vector of length 28, which can be accessed by various *output commands*. The scalar is the magnitude of the bias potential (energy units) applied on the current timestep, summed over all biased bonds. The vector stores the following quantities:

- 1 = average boost for all bonds on this step (unitless)
- 2 = # of biased bonds on this step
- 3 = max strain E_{ij} of any bond on this step (absolute value, unitless)

- 4 = value of V^{max} on this step (energy units)
- 5 = average bias coeff for all bonds on this step (unitless)
- 6 = min bias coeff for all bonds on this step (unitless)
- 7 = max bias coeff for all bonds on this step (unitless)
- 8 = average # of bonds/atom on this step
- 9 = average neighbor bonds/bond on this step within *Dcut*
- 10 = average boost for all bonds during this run (unitless)
- 11 = average # of biased bonds/step during this run
- 12 = fraction of biased bonds with no bias during this run
- 13 = fraction of biased bonds with negative strain during this run
- 14 = max bond length during this run (distance units)
- 15 = average bias coeff for all bonds during this run (unitless)
- 16 = min bias coeff for any bond during this run (unitless)
- 17 = max bias coeff for any bond during this run (unitless)
- 18 = max drift distance of any bond atom during this run (distance units)
- 19 = max distance from proc subbox of any ghost atom with maxstrain < qfactor during this run (distance units)
- 20 = max distance outside my box of any ghost atom with any maxstrain during this run (distance units)
- 21 = count of ghost atoms that could not be found on reneighbor steps during this run
- 22 = count of bias overlaps (< Dcut) found during this run
- 23 = cumulative hyper time since fix created (time units)
- 24 = cumulative count of event timesteps since fix created
- 25 = cumulative count of atoms in events since fix created
- 26 = cumulative # of new bonds formed since fix created

27 = average boost for biased bonds on this step (unitless) 28 = # of bonds with absolute strain >= q on this step

The first quantities 1-9 are for the current timestep. Quantities 10-22 are for the current hyper run. They are reset each time a new hyper run is performed. Quantities 23-26 are cumulative across multiple runs (since the point in the input script the fix was defined).

For value 10, each bond instantaneous boost factor is given by the equation for B_{ij} above. The total system boost (average across all bonds) fluctuates, but should average to a value close to the specified B_{target}.

For value 12, the numerator is a count of all biased bonds on each timestep whose bias energy = 0.0 due to $E_{ij} >= qfactor$. The denominator is the count of all biased bonds on all timesteps.

For value 13, the numerator is a count of all biased bonds on each timestep with negative strain. The denominator is the count of all biased bonds on all timesteps.

Values 18-22 are mostly useful for debugging and diagnostic purposes.

For value 18, drift is the distance an atom moves between two quenched states when the second quench determines an event has occurred. Atoms involved in an event will typically move the greatest distance since others typically remain near their original quenched position.

For values 19-21, neighbor atoms in the full neighbor list with cutoff *Dcut* may be ghost atoms outside a processor's sub-box. Before the next event occurs they may move further than *Dcut* away from the sub-box boundary. Value 19

is the furthest (from the sub-box) any ghost atom in the neighbor list with maxstrain < *qfactor* was accessed during the run. Value 20 is the same except that the ghost atom's maxstrain may be >= *qfactor*, which may mean it is about to participate in an event. Value 21 is a count of how many ghost atoms could not be found on reneighbor steps, presumably because they moved too far away due to their participation in an event (which will likely be detected at the next quench).

Typical values for 19 and 20 should be slightly larger than *Dcut*, which accounts for ghost atoms initially at a *Dcut* distance moving thermally before the next event takes place.

Note that for values 19 and 20 to be computed, the optional keyword *check/ghost* must be specified. Otherwise these values will be zero. This is because computing them incurs overhead, so the values are only computed if requested.

Value 21 should be zero or small. As explained above a small count likely means some ghost atoms were participating in their own events and moved a longer distance. If the value is large, it likely means the communication cutoff for ghosts is too close to *Dcut* leading to many not-found ghost atoms before the next event. This may lead to a reduced number of bonds being selected for biasing, since the code assumes those atoms are part of highly strained bonds. As explained above, the *comm_modify cutoff* command can be used to set a longer cutoff.

For value 22, no two bonds should be biased if they are within a *Dcut* distance of each other. This value should be zero, indicating that no pair of biased bonds are closer than *Dcut* from each other.

Note that for value 22 to be computed, the optional keyword *check/bias* must be specified and it determines how often this check is performed. This is because performing the check incurs overhead, so if only computed as often as requested.

The result at the end of the run is the cumulative total from every timestep the check was made. Note that the value is a count of atoms in bonds which found other atoms in bonds too close, so it is almost always an over-count of the number of too-close bonds.

Value 23 is simply the specified *boost* factor times the number of timesteps times the timestep size.

For value 24, events are checked for by the *hyper* command once every *Nevent* timesteps. This value is the count of those timesteps on which one (or more) events was detected. It is NOT the number of distinct events, since more than one event may occur in the same *Nevent* time window.

For value 25, each time the *hyper* command checks for an event, it invokes a compute to flag zero or more atoms as participating in one or more events. E.g. atoms that have displaced more than some distance from the previous quench state. Value 25 is the cumulative count of the number of atoms participating in any of the events that were found.

Value 26 tallies the number of new bonds created by the bond reset operation. Bonds between a specific I,J pair of atoms may persist for the entire hyperdynamics simulation if neither I or J are involved in an event.

Value 27 computes the average boost for biased bonds only on this step.

Value 28 is the count of bonds with an absolute value of strain >= q on this step.

The scalar and vector values calculated by this fix are all "intensive".

This fix also computes a local vector of length the number of bonds currently in the system. The value for each bond is its C_{ij} prefactor (bias coefficient). These values can be can be accessed by various *output commands*. A particularly useful one is the *fix ave/histo* command which can be used to histogram the Cij values to see if they are distributed reasonably close to 1.0, which indicates a good choice of V^{max}.

The local values calculated by this fix are unitless.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.65.4 Restrictions

This fix is part of the REPLICA package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.65.5 Related commands

hyper, *fix hyper/global*

16.65.6 Default

The default settings for optimal keywords are bounds = -1 and reset = -1. The check/ghost and check/bias keywords are not enabled by default.

(Voter2013) S. Y. Kim, D. Perez, A. F. Voter, J Chem Phys, 139, 144110 (2013).

(Miron) R. A. Miron and K. A. Fichthorn, J Chem Phys, 119, 6210 (2003).

16.66 fix imd command

16.66.1 Syntax

```
fix ID group-ID imd trate port keyword values ...
```

- ID, group-ID are documented in *fix* command
- imd = style name of this fix command
- port = port number on which the fix listens for an IMD client
- keyword = *unwrap* or *fscale* or *trate*

```
unwrap arg = on or off
  off = coordinates are wrapped back into the principal unit cell␣
↪(default)
  on = "unwrapped" coordinates using the image flags used
fscale arg = factor
  factor = floating point number to scale IMD forces (default: 1.0)
trate arg = transmission rate of coordinate data sets (default: 1)
nowait arg = on or off
  off = LAMMPS waits to be connected to an IMD client before continuing␣
↪(default)
  on = LAMMPS listens for an IMD client, but continues with the run
```

16.66.2 Examples

```
fix vmd all imd 5678
fix comm all imd 8888 trate 5 unwrap on fscale 10.0
```

16.66.3 Description

This fix implements the "Interactive MD" (IMD) protocol which allows realtime visualization and manipulation of MD simulations through the IMD protocol, as initially implemented in VMD and NAMD. Specifically it allows LAMMPS to connect an IMD client, for example the VMD visualization program, so that it can monitor the progress of the simulation and interactively apply forces to selected atoms.

If LAMMPS is compiled with the pre-processor flag -DLAMMPS_ASYNC_IMD then fix imd will use POSIX threads to spawn a IMD communication thread on MPI rank 0 in order to offload data reading and writing from the main execution thread and potentially lower the inferred latencies for slow communication links. This feature has only been tested under linux.

There are example scripts for using this package with LAMMPS in examples/USER/imd. Additional examples and a driver for use with the Novint Falcon game controller as haptic device can be found at: http://sites.google.com/site/akohlmey/software/vrpn-icms.

The source code for this fix includes code developed by the Theoretical and Computational Biophysics Group in the Beckman Institute for Advanced Science and Technology at the University of Illinois at Urbana-Champaign. We thank them for providing a software interface that allows codes like LAMMPS to hook to VMD.

Upon initialization of the fix, it will open a communication port on the node with MPI task 0 and wait for an incoming connection. As soon as an IMD client is connected, the simulation will continue and the fix will send the current coordinates of the fix's group to the IMD client at every trate MD step. When using r-RESPA, trate applies to the steps of the outmost RESPA level. During a run with an active IMD connection also the IMD client can request to apply forces to selected atoms of the fix group.

The port number selected must be an available network port number. On many machines, port numbers < 1024 are reserved for accounts with system manager privilege and specific applications. If multiple imd fixes would be active at the same time, each needs to use a different port number.

The *nowait* keyword controls the behavior of the fix when no IMD client is connected. With the default setting of *off*, LAMMPS will wait until a connection is made before continuing with the execution. Setting *nowait* to *on* will have the LAMMPS code be ready to connect to a client, but continue with the simulation. This can for example be used to monitor the progress of an ongoing calculation without the need to be permanently connected or having to download a trajectory file.

The *trate* keyword allows to select how often the coordinate data is sent to the IMD client. It can also be changed on request of the IMD client through an IMD protocol message. The *unwrap* keyword allows to send "unwrapped" coordinates to the IMD client that undo the wrapping back of coordinates into the principle unit cell, as done by default in LAMMPS. The *fscale* keyword allows to apply a scaling factor to forces transmitted by the IMD client. The IMD protocols stipulates that forces are transferred in kcal/mol/angstrom under the assumption that coordinates are given in angstrom. For LAMMPS runs with different units or as a measure to tweak the forces generated by the manipulation of the IMD client, this option allows to make adjustments.

To connect VMD to a listening LAMMPS simulation on the same machine with fix imd enabled, one needs to start VMD and load a coordinate or topology file that matches the fix group. When the VMD command prompts appears, one types the command line:

```
imd connect localhost 5678
```

This assumes that *fix imd* was started with 5678 as a port number for the IMD protocol.

The steps to do interactive manipulation of a running simulation in VMD are the following:

In the Mouse menu of the VMD Main window, select "Mouse -> Force -> Atom". You may alternately select "Residue", or "Fragment" to apply forces to whole residues or fragments. Your mouse can now be used to apply forces to your simulation. Click on an atom, residue, or fragment and drag to apply a force. Click quickly without moving the mouse to turn the force off. You can also use a variety of 3D position trackers to apply forces to your simulation. Game controllers or haptic devices with force-feedback such as the Novint Falcon or Sensable PHANTOM allow you to feel the resistance due to inertia or interactions with neighbors that the atoms experience you are trying to move, as if they were real objects. See the VMD IMD Homepage and the VRPN-ICMS Homepage for more details.

If IMD control messages are received, a line of text describing the message and its effect will be printed to the LAMMPS output screen, if screen output is active.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global scalar or vector or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.66.4 Restrictions

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

When used in combination with VMD, a topology or coordinate file has to be loaded, which matches (in number and ordering of atoms) the group the fix is applied to. The fix internally sorts atom IDs by ascending integer value; in VMD (and thus the IMD protocol) those will be assigned 0-based consecutive index numbers.

When using multiple active IMD connections at the same time, each needs to use a different port number.

Related commands: none

Default: none

16.67 fix indent command

16.67.1 Syntax

```
fix ID group-ID indent K keyword values ...
```

- ID, group-ID are documented in *fix* command
- indent = style name of this fix command
- K = force constant for indenter surface (force/distance^2 units)
- one or more keyword/value pairs may be appended
- keyword = *sphere* or *cylinder* or *plane* or *side* or *units*

```
sphere args = x y z R
  x,y,z = initial position of center of indenter (distance units)
  R = sphere radius of indenter (distance units)
  any of x,y,z,R can be a variable (see below)
cylinder args = dim c1 c2 R
  dim = x or y or z = axis of cylinder
```

```
    c1,c2 = coords of cylinder axis in other 2 dimensions (distance units)
    R = cylinder radius of indenter (distance units)
    any of c1,c2,R can be a variable (see below)
  plane args = dim pos side
    dim = x or y or z = plane perpendicular to this dimension
    pos = position of plane in dimension x, y, or z (distance units)
    pos can be a variable (see below)
    side = lo or hi
  side value = in or out
    in = the indenter acts on particles inside the sphere or cylinder
    out = the indenter acts on particles outside the sphere or cylinder
  units value = lattice or box
    lattice = the geometry is defined in lattice units
    box = the geometry is defined in simulation box units
```

16.67.2 Examples

```
fix 1 all indent 10.0 sphere 0.0 0.0 15.0 3.0
fix 1 all indent 10.0 sphere v_x v_y 0.0 v_radius side in
fix 2 flow indent 10.0 cylinder z 0.0 0.0 10.0 units box
```

16.67.3 Description

Insert an indenter within a simulation box. The indenter repels all atoms in the group that touch it, so it can be used to push into a material or as an obstacle in a flow. Or it can be used as a constraining wall around a simulation; see the discussion of the *side* keyword below.

The indenter can either be spherical or cylindrical or planar. You must set one of those 3 keywords.

A spherical indenter exerts a force of magnitude

```
F(r) = - K (r - R)^2
```

on each atom where K is the specified force constant, r is the distance from the atom to the center of the indenter, and R is the radius of the indenter. The force is repulsive and F(r) = 0 for $r > R$.

A cylindrical indenter exerts the same force, except that r is the distance from the atom to the center axis of the cylinder. The cylinder extends infinitely along its axis.

Spherical and cylindrical indenters account for periodic boundaries in two ways. First, the center point of a spherical indenter (x,y,z) or axis of a cylindrical indenter (c1,c2) is remapped back into the simulation box, if the box is periodic in a particular dimension. This occurs every timestep if the indenter geometry is specified with a variable (see below), e.g. it is moving over time. Second, the calculation of distance to the indenter center or axis accounts for periodic boundaries. Both of these mean that an indenter can effectively move through and straddle one or more periodic boundaries.

A planar indenter is really an axis-aligned infinite-extent wall exerting the same force on atoms in the system, where R is the position of the plane and r-R is the distance from the plane. If the *side* parameter of the plane is specified as *lo* then it will indent from the lo end of the simulation box, meaning that atoms with a coordinate less than the plane's current position will be pushed towards the hi end of the box and atoms with a coordinate higher than the plane's current position will feel no force. Vice versa if *side* is specified as *hi*.

Any of the 4 quantities defining a spherical indenter's geometry can be specified as an equal-style *variable*, namely x, y, z, or R. Similarly, for a cylindrical indenter, any of *c1*, *c2*, or R, can be a variable. For a planar indenter, *pos* can be a variable. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to define the indenter geometry.

Note that equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify indenter properties that change as a function of time or span consecutive runs in a continuous fashion. For the latter, see the *start* and *stop* keywords of the *run* command and the *elaplong* keyword of *thermo_style custom* for details.

For example, if a spherical indenter's x-position is specified as v_x, then this variable definition will keep it's center at a relative position in the simulation box, 1/4 of the way from the left edge to the right edge, even if the box size changes:

```
variable x equal "xlo + 0.25*lx"
```

Similarly, either of these variable definitions will move the indenter from an initial position at 2.5 at a constant velocity of 5:

```
variable x equal "2.5 + 5*elaplong*dt"
variable x equal vdisplace(2.5,5)
```

If a spherical indenter's radius is specified as v_r, then these variable definitions will grow the size of the indenter at a specified rate.

```
variable r0 equal 0.0
variable rate equal 1.0
variable r equal "v_r0 + step*dt*v_rate"
```

If the *side* keyword is specified as *out*, which is the default, then particles outside the indenter are pushed away from its outer surface, as described above. This only applies to spherical or cylindrical indenters. If the *side* keyword is specified as *in*, the action of the indenter is reversed. Particles inside the indenter are pushed away from its inner surface. In other words, the indenter is now a containing wall that traps the particles inside it. If the radius shrinks over time, it will squeeze the particles.

The *units* keyword determines the meaning of the distance units used to define the indenter geometry. A *box* value selects standard distance units as defined by the *units* command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacing. The (x,y,z) coords of the indenter position are scaled by the x,y,z lattice spacings respectively. The radius of a spherical or cylindrical indenter is scaled by the x lattice spacing.

Note that the units keyword only affects indenter geometry parameters specified directly with numbers, not those specified as variables. In the latter case, you should use the *xlat*, *ylat*, *zlat* keywords of the *thermo_style* command if you want to include lattice spacings in a variable formula.

The force constant *K* is not affected by the *units* keyword. It is always in force/distance^2 units where force and distance are defined by the *units* command. If you wish K to be scaled by the lattice spacing, you can define K with a variable whose formula contains *xlat*, *ylat*, *zlat* keywords of the *thermo_style* command, e.g.

```
variable k equal 100.0/xlat/xlat
fix 1 all indent $k sphere ...
```

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify energy* option is supported by this fix to add the energy of interaction between atoms and the indenter to the system's potential energy as part of *thermodynamic output*. The energy of each particle interacting with the indenter is K/3 (r - R)^3.

The *fix_modify respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix is adding its forces. Default is the outermost level.

This fix computes a global scalar energy and a global 3-vector of forces (on the indenter), which can be accessed by various *output commands*. The scalar and vector values calculated by this fix are "extensive".

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command. Note that if you define the indenter geometry with a variable using a time-dependent formula, LAMMPS uses the iteration count in the minimizer as the timestep. But it is almost certainly a bad idea to have the indenter change its position or size during a minimization. LAMMPS does not check if you have done this.

Note: If you want the atom/indenter interaction energy to be included in the total potential energy of the system (the quantity being minimized), you must enable the *fix_modify energy* option for this fix.

16.67.4 Restrictions

none

Related commands: none

16.67.5 Default

The option defaults are side = out and units = lattice.

16.68 fix ipi command

16.68.1 Syntax

```
fix ID group-ID ipi address port [unix] [reset]
```

- ID, group-ID are documented in *fix* command
- ipi = style name of this fix command
- address = internet address (FQDN or IP), or UNIX socket name
- port = port number (ignored for UNIX sockets)
- optional keyword = *unix*, if present uses a unix socket
- optional keyword = *reset*, if present reset electrostatics at each call

16.68.2 Examples

fix 1 all ipi my.server.com 12345 fix 1 all ipi mysocket 666 unix reset

16.68.3 Description

This fix enables LAMMPS to be run as a client for the i-PI Python wrapper *(IPI)* for performing a path integral molecular dynamics (PIMD) simulation. The philosophy behind i-PI is described in the following publication *(IPI-CPC)*.

A version of the i-PI package, containing only files needed for use with LAMMPS, is provided in the tools/i-pi directory. See the tools/i-pi/manual.pdf for an introduction to i-PI. The examples/USER/i-pi directory contains example scripts for using i-PI with LAMMPS.

In brief, the path integral molecular dynamics is performed by the Python wrapper, while the client (LAMMPS in this case) simply computes forces and energy for each configuration. The communication between the two components takes place using sockets, and is reduced to the bare minimum. All the parameters of the dynamics are specified in the input of i-PI, and all the parameters of the force field must be specified as LAMMPS inputs, preceding the *fix ipi* command.

The server address must be specified by the *address* argument, and can be either the IP address, the fully-qualified name of the server, or the name of a UNIX socket for local, faster communication. In the case of internet sockets, the *port* argument specifies the port number on which i-PI is listening, while the *unix* optional switch specifies that the socket is a UNIX socket.

Note that there is no check of data integrity, or that the atomic configurations make sense. It is assumed that the species in the i-PI input are listed in the same order as in the data file of LAMMPS. The initial configuration is ignored, as it will be substituted with the coordinates received from i-PI before forces are ever evaluated.

A note of caution when using potentials that contain long-range electrostatics, or that contain parameters that depend on box size: all of these options will be initialized based on the cell size in the LAMMPS-side initial configuration and kept constant during the run. This is required to e.g. obtain reproducible and conserved forces. If the cell varies too wildly, it may be advisable to re-initialize these interactions at each call. This behavior can be requested by setting the *reset* switch.

Restart, fix_modify, output, run start/stop, minimize info:

There is no restart information associated with this fix, since all the dynamical parameters are dealt with by i-PI.

16.68.4 Restrictions

Using this fix on anything other than all atoms requires particular care, since i-PI will know nothing on atoms that are not those whose coordinates are transferred. However, one could use this strategy to define an external potential acting on the atoms that are moved by i-PI.

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info. Because of the use of UNIX domain sockets, this fix will only work in a UNIX environment.

16.68.5 Related commands

fix nve

(IPI-CPC) Ceriotti, More and Manolopoulos, Comp Phys Comm, 185, 1019-1026 (2014).

(IPI) http://epfl-cosmo.github.io/gle4md/index.html?page=ipi

16.69 fix langevin command

16.70 fix langevin/kk command

16.70.1 Syntax

```
fix ID group-ID langevin Tstart Tstop damp seed keyword values ...
```

- ID, group-ID are documented in *fix* command

- langevin = style name of this fix command
- Tstart,Tstop = desired temperature at start/end of run (temperature units)
- Tstart can be a variable (see below)
- damp = damping parameter (time units)
- seed = random number seed to use for white noise (positive integer)
- zero or more keyword/value pairs may be appended
- keyword = *angmom* or *omega* or *scale* or *tally* or *zero*

```
angmom value = no or factor
  no = do not thermostat rotational degrees of freedom via the angular␣
↪momentum
  factor = do thermostat rotational degrees of freedom via the angular␣
↪momentum and apply numeric scale factor as discussed below
gjf value = no or vfull or vhalf
  no = use standard formulation
  vfull = use Gronbech-Jensen/Farago formulation
  vhalf = use 2GJ formulation
omega value = no or yes
  no = do not thermostat rotational degrees of freedom via the angular␣
↪velocity
  yes = do thermostat rotational degrees of freedom via the angular␣
↪velocity
scale values = type ratio
  type = atom type (1-N)
  ratio = factor by which to scale the damping coefficient
tally value = no or yes
  no = do not tally the energy added/subtracted to atoms
  yes = do tally the energy added/subtracted to atoms
zero value = no or yes
  no = do not set total random force to zero
  yes = set total random force to zero
```

16.70.2 Examples

```
fix 3 boundary langevin 1.0 1.0 1000.0 699483
fix 1 all langevin 1.0 1.1 100.0 48279 scale 3 1.5
fix 1 all langevin 1.0 1.1 100.0 48279 angmom 3.333
```

16.70.3 Description

Apply a Langevin thermostat as described in *(Schneider)* to a group of atoms which models an interaction with a background implicit solvent. Used with *fix nve*, this command performs Brownian dynamics (BD), since the total force on each atom will have the form:

$$F = F_c + F_f + F_r$$
$$F_f = -\frac{m}{\text{damp}} v$$
$$F_r \propto \sqrt{\frac{k_B T m}{dt\ \text{damp}}}$$

F_c is the conservative force computed via the usual inter-particle interactions (*pair_style*, *bond_style*, etc). The F_f and F_r terms are added by this fix on a per-particle basis. See the *pair_style dpd/tstat* command for a thermostatting option that adds similar terms on a pairwise basis to pairs of interacting particles.

F_f is a frictional drag or viscous damping term proportional to the particle's velocity. The proportionality constant for each atom is computed as $\frac{m}{\mathrm{damp}}$, where *m* is the mass of the particle and damp is the damping factor specified by the user.

F_r is a force due to solvent atoms at a temperature *T* randomly bumping into the particle. As derived from the fluctuation/dissipation theorem, its magnitude as shown above is proportional to $\sqrt{\frac{k_B T m}{dt\ \mathrm{damp}}}$, where k_B is the Boltzmann constant, *T* is the desired temperature, *m* is the mass of the particle, *dt* is the timestep size, and damp is the damping factor. Random numbers are used to randomize the direction and magnitude of this force as described in *(Dunweg)*, where a uniform random number is used (instead of a Gaussian random number) for speed.

Note that unless you use the *omega* or *angmom* keywords, the thermostat effect of this fix is applied to only the translational degrees of freedom for the particles, which is an important consideration for finite-size particles, which have rotational degrees of freedom, are being thermostatted. The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

Note: Unlike the *fix nvt* command which performs Nose/Hoover thermostatting AND time integration, this fix does NOT perform time integration. It only modifies forces to effect thermostatting. Thus you must use a separate time integration fix, like *fix nve* to actually update the velocities and positions of atoms using the modified forces. Likewise, this fix should not normally be used on atoms that also have their temperature controlled by another fix - e.g. by *fix nvt* or *fix temp/rescale* commands.

See the *Howto thermostat* doc page for a discussion of different ways to compute temperature and perform thermostatting.

The desired temperature at each timestep is a ramped value during the run from *Tstart* to *Tstop*.

Tstart can be specified as an equal-style or atom-style *variable*. In this case, the *Tstop* setting is ignored. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the target temperature.

Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent temperature.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent temperature with optional time-dependence as well.

Like other fixes that perform thermostatting, this fix can be used with *compute commands* that remove a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or removing the x-component of velocity from the calculation. This is not done by default, but only if the *fix_modify* command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual *compute commands* to determine which ones include a bias. In this case, the thermostat works in the following manner: bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

The *damp* parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 100.0 means to relax the temperature in a timespan of (roughly) 100 time units (τ or fs or ps - see the *units* command). The damp factor can be thought of as inversely related to the viscosity of the solvent. I.e. a small relaxation time implies a high-viscosity solvent and vice versa. See the discussion about γ and viscosity in the documentation for the *fix viscous* command for more details.

The random # *seed* must be a positive integer. A Marsaglia random number generator is used. Each processor uses the input seed to generate its own unique seed and its own stream of random numbers. Thus the dynamics of the system

will not be identical on two runs on different numbers of processors.

The keyword/value option pairs are used in the following ways.

The keyword *angmom* and *omega* keywords enable thermostatting of rotational degrees of freedom in addition to the usual translational degrees of freedom. This can only be done for finite-size particles.

A simulation using atom_style sphere defines an omega for finite-size spheres. A simulation using atom_style ellipsoid defines a finite size and shape for aspherical particles and an angular momentum. The Langevin formulas for thermostatting the rotational degrees of freedom are the same as those above, where force is replaced by torque, m is replaced by the moment of inertia I, and v is replaced by omega (which is derived from the angular momentum in the case of aspherical particles).

The rotational temperature of the particles can be monitored by the *compute temp/sphere* and *compute temp/asphere* commands with their rotate options.

For the *omega* keyword there is also a scale factor of $\frac{10.0}{3.0}$ that is applied as a multiplier on the F_f (damping) term in the equation above and of $\sqrt{\frac{10.0}{3.0}}$ as a multiplier on the F_r term. This does not affect the thermostatting behavior of the Langevin formalism but insures that the randomized rotational diffusivity of spherical particles is correct.

For the *angmom* keyword a similar scale factor is needed which is $\frac{10.0}{3.0}$ for spherical particles, but is anisotropic for aspherical particles (e.g. ellipsoids). Currently LAMMPS only applies an isotropic scale factor, and you can choose its magnitude as the specified value of the *angmom* keyword. If your aspherical particles are (nearly) spherical than a value of $\frac{10.0}{3.0} = 3.\overline{3}$ is a good choice. If they are highly aspherical, a value of 1.0 is as good a choice as any, since the effects on rotational diffusivity of the particles will be incorrect regardless. Note that for any reasonable scale factor, the thermostatting effect of the *angmom* keyword on the rotational temperature of the aspherical particles should still be valid.

The keyword *scale* allows the damp factor to be scaled up or down by the specified factor for atoms of that type. This can be useful when different atom types have different sizes or masses. It can be used multiple times to adjust damp for several atom types. Note that specifying a ratio of 2 increases the relaxation time which is equivalent to the solvent's viscosity acting on particles with $\frac{1}{2}$ the diameter. This is the opposite effect of scale factors used by the *fix viscous* command, since the damp factor in fix *langevin* is inversely related to the γ factor in fix *viscous*. Also note that the damping factor in fix *langevin* includes the particle mass in Ff, unlike fix *viscous*. Thus the mass and size of different atom types should be accounted for in the choice of ratio values.

The keyword *tally* enables the calculation of the cumulative energy added/subtracted to the atoms as they are thermostatted. Effectively it is the energy exchanged between the infinite thermal reservoir and the particles. As described below, this energy can then be printed out or added to the potential energy of the system to monitor energy conservation.

Note: this accumulated energy does NOT include kinetic energy removed by the *zero* flag. LAMMPS will print a warning when both options are active.

The keyword *zero* can be used to eliminate drift due to the thermostat. Because the random forces on different atoms are independent, they do not sum exactly to zero. As a result, this fix applies a small random force to the entire system, and the center-of-mass of the system undergoes a slow random walk. If the keyword *zero* is set to *yes*, the total random force is set exactly to zero by subtracting off an equal part of it from each atom in the group. As a result, the center-of-mass of a system with zero initial momentum will not drift over time.

The keyword *gjf* can be used to run the *Gronbech-Jensen/Farago* time-discretization of the Langevin model. As described in the papers cited below, the purpose of this method is to enable longer timesteps to be used (up to the numerical stability limit of the integrator), while still producing the correct Boltzmann distribution of atom positions.

The current implementation provides the user with the option to output the velocity in one of two forms: *vfull* or *vhalf*, which replaces the outdated option *yes*. The *gjf* option *vfull* outputs the on-site velocity given in *Gronbech-*

Jensen/Farago; this velocity is shown to be systematically lower than the target temperature by a small amount, which grows quadratically with the timestep. The *gjf* option *vhalf* outputs the 2GJ half-step velocity given in *Gronbech Jensen/Gronbech-Jensen*; for linear systems, this velocity is shown to not have any statistical errors for any stable time step. An overview of statistically correct Boltzmann and Maxwell-Boltzmann sampling of true on-site and true half-step velocities is given in *Gronbech-Jensen*. Regardless of the choice of output velocity, the sampling of the configurational distribution of atom positions is the same, and linearly consistent with the target temperature.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior.

The *fix_modify* *temp* option is supported by this fix. You can use it to assign a temperature *compute* you have defined to this fix which will be used in its thermostatting procedure, as described above. For consistency, the group used by this fix and by the compute should be the same.

The *fix_modify* *energy* option is supported by this fix to add the energy change induced by Langevin thermostatting to the system's potential energy as part of *thermodynamic output*. Note that use of this option requires setting the *tally* keyword to *yes*.

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the cumulative energy change due to this fix. The scalar value calculated by this fix is "extensive". Note that calculation of this quantity requires setting the *tally* keyword to *yes*.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.70.4 Restrictions

For *gjf* do not choose damp=dt/2. *gjf* is not compatible with run_style respa.

16.70.5 Related commands

fix nvt, *fix temp/rescale*, *fix viscous*, *fix nvt*, *pair_style dpd/tstat*

16.70.6 Default

The option defaults are angmom = no, omega = no, scale = 1.0 for all types, tally = no, zero = no, gjf = no.

(Dunweg) Dunweg and Paul, Int J of Modern Physics C, 2, 817-27 (1991).

(Schneider) Schneider and Stoll, Phys Rev B, 17, 1302 (1978).

(Gronbech-Jensen) Gronbech-Jensen and Farago, Mol Phys, 111, 983 (2013); Gronbech-Jensen, Hayre, and Farago, Comp Phys Comm, 185, 524 (2014)

(Gronbech-Jensen) Gronbech Jensen and Gronbech-Jensen, Mol Phys, 117, 2511 (2019)

(Gronbech-Jensen) Gronbech-Jensen, Mol Phys (2019); https://doi.org/10.1080/00268976.2019.1662506

16.71 fix langevin/drude command

16.71.1 Syntax

```
fix ID group-ID langevin/drude Tcom damp_com seed_com Tdrude damp_drude seed_drude␣
↪keyword values ...
```

- ID, group-ID are documented in *fix* command
- langevin/drude = style name of this fix command
- Tcom = desired temperature of the centers of mass (temperature units)
- damp_com = damping parameter for the thermostat on centers of mass (time units)
- seed_com = random number seed to use for white noise of the thermostat on centers of mass (positive integer)
- Tdrude = desired temperature of the Drude oscillators (temperature units)
- damp_drude = damping parameter for the thermostat on Drude oscillators (time units)
- seed_drude = random number seed to use for white noise of the thermostat on Drude oscillators (positive integer)
- zero or more keyword/value pairs may be appended
- keyword = *zero*

  ```
  zero value = no or yes
    no = do not set total random force on centers of mass to zero
    yes = set total random force on centers of mass to zero
  ```

16.71.2 Examples

```
fix 3 all langevin/drude 300.0 100.0 19377 1.0 20.0 83451
fix 1 all langevin/drude 298.15 100.0 19377 5.0 10.0 83451 zero yes
```

16.71.3 Description

Apply two Langevin thermostats as described in *(Jiang)* for thermalizing the reduced degrees of freedom of Drude oscillators. This link describes how to use the *thermalized Drude oscillator model* in LAMMPS and polarizable models in LAMMPS are discussed on the *Howto polarizable* doc page.

Drude oscillators are a way to simulate polarizables atoms, by splitting them into a core and a Drude particle bound by a harmonic bond. The thermalization works by transforming the particles degrees of freedom by these equations. In these equations upper case denotes atomic or center of mass values and lower case denotes Drude particle or dipole values. Primes denote the transformed (reduced) values, while bare letters denote the original values.

Velocities:

$$V' = \frac{M\,V + m\,v}{M'}$$

$$v' = v - V$$

Masses:

$$M' = M + m$$

$$m' = \frac{M\,m}{M'}$$

The Langevin forces are computed as

$$F' = -\frac{M'}{\texttt{damp_com}}\,V' + F'_r$$

$$f' = -\frac{m'}{\texttt{damp_drude}}\,v' + f'_r$$

F'_r is a random force proportional to $\sqrt{\frac{2\,k_B \texttt{Tcom}\,m'}{\mathrm{d}t\,\texttt{damp_com}}}$. f'_r is a random force proportional to $\sqrt{\frac{2\,k_B \texttt{Tdrude}\,m'}{\mathrm{d}t\,\texttt{damp_drude}}}$. Then the real forces acting on the particles are computed from the inverse transform:

$$F = \frac{M}{M'}\,F' - f'$$

$$f = \frac{m}{M'}\,F' + f'$$

This fix also thermostats non-polarizable atoms in the group at temperature *Tcom*, as if they had a massless Drude partner. The Drude particles themselves need not be in the group. The center of mass and the dipole are thermostatted iff the core atom is in the group.

Note that the thermostat effect of this fix is applied to only the translational degrees of freedom of the particles, which is an important consideration if finite-size particles, which have rotational degrees of freedom, are being thermostatted. The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

Note: Like the *fix langevin* command, this fix does NOT perform time integration. It only modifies forces to effect thermostatting. Thus you must use a separate time integration fix, like *fix nve* or *fix nph* to actually update the velocities

and positions of atoms using the modified forces. Likewise, this fix should not normally be used on atoms that also have their temperature controlled by another fix - e.g. by *fix nvt* or *fix temp/rescale* commands.

See the *Howto thermostat* doc page for a discussion of different ways to compute temperature and perform thermostatting.

This fix requires each atom know whether it is a Drude particle or not. You must therefore use the *fix drude* command to specify the Drude status of each atom type.

Note: only the Drude core atoms need to be in the group specified for this fix. A Drude electron will be transformed together with its cores even if it is not itself in the group. It is safe to include Drude electrons or non-polarizable atoms in the group. The non-polarizable atoms will simply be thermostatted as if they had a massless Drude partner (electron).

Note: Ghost atoms need to know their velocity for this fix to act correctly. You must use the *comm_modify* command to enable this, e.g.

```
comm_modify vel yes
```

Tcom is the target temperature of the centers of mass, which would be used to thermostat the non-polarizable atoms. *Tdrude* is the (normally low) target temperature of the core-Drude particle pairs (dipoles). *Tcom* and *Tdrude* can be specified as an equal-style *variable*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the target temperature.

Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent temperature.

Like other fixes that perform thermostatting, this fix can be used with *compute commands* that remove a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms. This is not done by default, but only if the *fix_modify* command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual *compute commands* to determine which ones include a bias. In this case, the thermostat works in the following manner: bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in. NOTE: this feature has not been tested.

Note: The temperature thermostatting the core-Drude particle pairs should be chosen low enough, so as to mimic as closely as possible the self-consistent minimization. It must however be high enough, so that the dipoles can follow the local electric field exerted by the neighboring atoms. The optimal value probably depends on the temperature of the centers of mass and on the mass of the Drude particles.

damp_com is the characteristic time for reaching thermal equilibrium of the centers of mass. For example, a value of 100.0 means to relax the temperature of the centers of mass in a timespan of (roughly) 100 time units (tau or fmsec or psec - see the *units* command). *damp_drude* is the characteristic time for reaching thermal equilibrium of the dipoles. It is typically a few timesteps.

The number *seed_com* and *seed_drude* are positive integers. They set the seeds of the Marsaglia random number generators used for generating the random forces on centers of mass and on the dipoles. Each processor uses the input seed to generate its own unique seed and its own stream of random numbers. Thus the dynamics of the system will not be identical on two runs on different numbers of processors.

The keyword *zero* can be used to eliminate drift due to the thermostat on centers of mass. Because the random forces on different centers of mass are independent, they do not sum exactly to zero. As a result, this fix applies a small random force to the entire system, and the momentum of the total center of mass of the system undergoes a slow random walk. If the keyword *zero* is set to *yes*, the total random force on the centers of mass is set exactly to zero by subtracting off an equal part of it from each center of mass in the group. As a result, the total center of mass of a system with zero initial momentum will not drift over time.

The actual temperatures of cores and Drude particles, in center-of-mass and relative coordinates, respectively, can be calculated using the *compute temp/drude* command.

Usage example for rigid bodies in the NPT ensemble:

```
comm_modify vel yes
fix TEMP all langevin/drude 300. 100. 1256 1. 20. 13977 zero yes
fix NPH ATOMS rigid/nph/small molecule iso 1. 1. 500.
fix NVE DRUDES nve
compute TDRUDE all temp/drude
thermo_style custom step cpu etotal ke pe ebond ecoul elong press vol temp c_
↪TDRUDE[1] c_TDRUDE[2]
```

Comments:

- Drude particles should not be in the rigid group, otherwise the Drude oscillators will be frozen and the system will lose its polarizability.
- *zero yes* avoids a drift of the center of mass of the system, but is a bit slower.
- Use two different random seeds to avoid unphysical correlations.
- Temperature is controlled by the fix *langevin/drude*, so the time-integration fixes do not thermostat. Don't forget to time-integrate both cores and Drude particles.
- Pressure is time-integrated only once by using *nve* for Drude particles and *nph* for atoms/cores (or vice versa). Do not use *nph* for both.
- The temperatures of cores and Drude particles are calculated by *compute temp/drude*
- Contrary to the alternative thermostatting using Nose-Hoover thermostat fix *npt* and *fix drude/transform*, the *fix_modify* command is not required here, because the fix *nph* computes the global pressure even if its group is *ATOMS*. This is what we want. If we thermostatted *ATOMS* using *npt*, the pressure should be the global one, but the temperature should be only that of the cores. That's why the command *fix_modify* should be called in that case.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior.

The *fix_modify temp* option is supported by this fix. You can use it to assign a temperature *compute* you have defined to this fix which will be used in its thermostatting procedure, as described above. For consistency, the group used by the compute should include the group of this fix and the Drude particles.

This fix is not invoked during *energy minimization*.

16.71.4 Restrictions

none

16.71.5 Related commands

fix langevin, *fix drude*, *fix drude/transform*, *compute temp/drude*, *pair_style thole*

16.71.6 Default

The option defaults are zero = no.

(Jiang) Jiang, Hardy, Phillips, MacKerell, Schulten, and Roux, J Phys Chem Lett, 2, 87-92 (2011).

16.72 fix langevin/eff command

16.72.1 Syntax

```
fix ID group-ID langevin/eff Tstart Tstop damp seed keyword values ...
```

- ID, group-ID are documented in *fix* command
- langevin/eff = style name of this fix command
- Tstart,Tstop = desired temperature at start/end of run (temperature units)
- damp = damping parameter (time units)
- seed = random number seed to use for white noise (positive integer)
- zero or more keyword/value pairs may be appended

```
keyword = scale or tally or zero
  scale values = type ratio
    type = atom type (1-N)
    ratio = factor by which to scale the damping coefficient
  tally values = no or yes
    no = do not tally the energy added/subtracted to atoms
    yes = do tally the energy added/subtracted to atoms
zero value = no or yes
  no = do not set total random force to zero
  yes = set total random force to zero
```

16.72.2 Examples

```
fix 3 boundary langevin/eff 1.0 1.0 10.0 699483
fix 1 all langevin/eff 1.0 1.1 10.0 48279 scale 3 1.5
```

16.72.3 Description

Apply a Langevin thermostat as described in *(Schneider)* to a group of nuclei and electrons in the *electron force field* model. Used with *fix nve/eff*, this command performs Brownian dynamics (BD), since the total force on each atom will have the form:

$$
\begin{aligned}
F =& F_c + F_f + F_r \\
F_f =& -\frac{m}{\text{damp}} v \\
F_r \propto& \sqrt{\frac{k_B T m}{dt\ \text{damp}}}
\end{aligned}
$$

F_c is the conservative force computed via the usual inter-particle interactions (*pair_style*). The F_f and F_r terms are added by this fix on a per-particle basis.

The operation of this fix is exactly like that described by the *fix langevin* command, except that the thermostatting is also applied to the radial electron velocity for electron particles.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior.

The *fix_modify* *temp* option is supported by this fix. You can use it to assign a temperature *compute* you have defined to this fix which will be used in its thermostatting procedure, as described above. For consistency, the group used by this fix and by the compute should be the same.

The *fix_modify* *energy* option is supported by this fix to add the energy change induced by Langevin thermostatting to the system's potential energy as part of *thermodynamic output*. Note that use of this option requires setting the *tally* keyword to *yes*.

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the cumulative energy change due to this fix. The scalar value calculated by this fix is "extensive". Note that calculation of this quantity requires setting the *tally* keyword to *yes*.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.72.4 Restrictions

none

This fix is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.72.5 Related commands

fix langevin

16.72.6 Default

The option defaults are scale = 1.0 for all types and tally = no.

(Dunweg) Dunweg and Paul, Int J of Modern Physics C, 2, 817-27 (1991).

(Schneider) Schneider and Stoll, Phys Rev B, 17, 1302 (1978).

16.73 fix langevin/spin command

16.73.1 Syntax

```
fix ID group-ID langevin/spin T Tdamp seed
```

- ID, group-ID are documented in *fix* command
- langevin/spin = style name of this fix command
- T = desired temperature of the bath (temperature units, K in metal units)
- Tdamp = transverse magnetic damping parameter (adim)
- seed = random number seed to use for white noise (positive integer)

16.73.2 Examples

```
fix 2 all langevin/spin 300.0 0.01 21
```

16.73.3 Description

Apply a Langevin thermostat as described in *(Mayergoyz)* to the magnetic spins associated to the atoms. Used with *fix nve/spin*, this command performs Brownian dynamics (BD). A random torque and a transverse dissipation are applied to each spin i according to the following stochastic differential equation:

$$\frac{d\vec{s}_i}{dt} = \frac{1}{(1+\lambda^2)}\left((\vec{\omega}_i + \vec{\eta}) \times \vec{s}_i + \lambda\, \vec{s}_i \times (\vec{\omega}_i \times \vec{s}_i)\right)$$

with λ the transverse damping, and η a random vector. This equation is referred to as the stochastic Landau-Lifshitz-Gilbert (sLLG) equation.

The components of η are drawn from a Gaussian probability law. Their amplitude is defined as a proportion of the temperature of the external thermostat T (in K in metal units).

More details about this implementation are reported in *(Tranchida)*.

Note: due to the form of the sLLG equation, this fix has to be defined just before the nve/spin fix (and after all other magnetic fixes). As an example:

```
fix 1 all precession/spin zeeman 0.01 0.0 0.0 1.0
fix 2 all langevin/spin 300.0 0.01 21
fix 3 all nve/spin lattice moving
```

is correct, but defining a force/spin command after the langevin/spin command would give an error message.

Note: The random # *seed* must be a positive integer. A Marsaglia random number generator is used. Each processor uses the input seed to generate its own unique seed and its own stream of random numbers. Thus the dynamics of the system will not be identical on two runs on different numbers of processors.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior.

This fix is not invoked during *energy minimization*.

16.73.4 Restrictions

The *langevin/spin* fix is part of the SPIN package. This style is only enabled if LAMMPS was built with this package. See the *Build package* doc page for more info.

The numerical integration has to be performed with *fix nve/spin* when *fix langevin/spin* is enabled.

This fix has to be the last defined magnetic fix before the time integration fix (e.g. *fix nve/spin*).

16.73.5 Related commands

fix nve/spin, *fix precession/spin*

Default: none

(Mayergoyz) I.D. Mayergoyz, G. Bertotti, C. Serpico (2009). Elsevier (2009)

(Tranchida) Tranchida, Plimpton, Thibaudeau and Thompson, Journal of Computational Physics, 372, 406-425, (2018).

16.74 fix latte command

16.74.1 Syntax

```
fix ID group-ID latte peID
```

- ID, group-ID are documented in *fix* command
- latte = style name of this fix command
- peID = NULL or ID of compute used to calculate per-atom energy

16.74.2 Examples

```
fix dftb all latte NULL
```

16.74.3 Description

This fix style is a wrapper on the self-consistent charge transfer density functional based tight binding (DFTB) code LATTE. If you download and build LATTE, it can be called as a library by LAMMPS via this fix to run dynamics or perform energy minimization using DFTB forces and energies computed by LATTE.

LATTE is principally developed and supported by Marc Cawkwell and co-workers at Los Alamos National Laboratory (LANL). See the full list of contributors in the src/LATTE/README file.

To use this fix, the LATTE program needs to be compiled as a library and linked with LAMMPS. LATTE can be downloaded (or cloned) from https://github.com/lanl/LATTE. Instructions on how to download and build LATTE on your system can be found in the lib/latte/README. Note that you can also use the "make lib-latte" command from the LAMMPS src directory to automate this process.

Once LAMMPS is built with the LATTE package, you can run the example input scripts for molecular dynamics or energy minimization that are found in examples/latte.

A step-by-step tutorial can be followed at: LAMMPS-LATTE tutorial

The *peID* argument is not yet supported by fix latte, so it must be specified as NULL. Eventually it will be used to enable LAMMPS to calculate a Coulomb potential as an alternative to LATTE performing the calculation.

LATTE is a code for performing self-consistent charge transfer tight-binding (SC-TB) calculations of total energies and the forces acting on atoms in molecules and solids. This tight-binding method is becoming more and more popular and widely used in chemistry, biochemistry, material science, etc.

The SC-TB formalism is derived from an expansion of the Kohn-Sham density functional to second order in charge fluctuations about a reference charge of overlapping atom-centered densities and bond integrals are parameterized using a Slater-Koster tight-binding approach. This procedure, which usually is referred to as the DFTB method has been described in detail by (*Elstner*) and (*Finnis*) and coworkers.

The work of the LATTE developers follows that of Elstner closely with respect to the physical model. However, the development of LATTE is geared principally toward large-scale, long duration, microcanonical quantum-based Born-Oppenheimer molecular dynamics (QMD) simulations. One of the main bottlenecks of an electronic structure calculation is the solution of the generalized eigenvalue problem which scales with the cube of the system size O(N^3).

The Theoretical and Computer sciences divisions at Los Alamos National Laboratory have accumulated large experience addressing this issue by calculating the density matrix directly instead of using diagonalization. We typically use

a recursive sparse Fermi-operator expansion using second-order spectral projection functions (SP2-algorithm), which was introduced by Niklasson in 2002 (*Niklasson2002*), (*Rubensson*), (*Mniszewski*). When the matrices involved in the recursive expansion are sufficiently sparse, the calculation of the density matrix scales linearly as a function of the system size O(N).

Another important feature is the extended Lagrangian framework for Born-Oppenheimer molecular dynamics (XL-BOMD) (*Niklasson2008*) (*Niklasson2014*), (*Niklasson2017*) that allows for a drastic reduction or even a complete removal of the iterative self-consistent field optimization. Often only a single density matrix calculation per molecular dynamics time step is required, yet total energy stability is well maintained. The SP2 and XL-BOMD techniques enables stable linear scaling MD simulations with a very small computational overhead. This opens a number of opportunities in many different areas of chemistry and materials science, as we now can simulate larger system sizes and longer time scales (*Cawkwell2012*), (*Negre2016*).

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify* *energy* option is supported by this fix to add the potential energy computed by LATTE to the system's potential energy as part of *thermodynamic output*.

The *fix_modify* *virial* option is supported by this fix to add the LATTE DFTB contribution to the system's virial as part of *thermodynamic output*. The default is *virial yes*

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the potential energy discussed above. The scalar value calculated by this fix is "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The DFTB forces computed by LATTE via this fix are imposed during an energy minimization, invoked by the *minimize* command.

Note: If you want the potential energy associated with the DFTB forces to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the *fix_modify* *energy* option for this fix.

16.74.4 Restrictions

This fix is part of the LATTE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

You must use metal units, as set by the *units* command to use this fix.

LATTE does not currently compute per-atom energy or per-atom virial contributions. So they will not show up as part of the calculations performed by the *compute pe/atom* or *compute stress/atom* commands.

Currently, LAMMPS must be run in serial or as a single MPI task, to use this fix. This is typically not a bottleneck, since LATTE will be doing 99% or more of the work to compute quantum-accurate forces.

Note: NEB calculations can be done using this fix using multiple replicas and running LAMMPS in parallel. However, each replica must be run on a single MPI task. For details, see the *neb* command doc page and the *-partition command-line switch*

Related commands: none

Default: none

(Elstner) M. Elstner, D. Poresag, G. Jungnickel, J. Elsner, M. Haugk, T. Frauenheim, S. Suhai, and G. Seifert, Phys. Rev. B, 58, 7260 (1998).

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16.75 fix lb/fluid command

16.75.1 Syntax

```
fix ID group-ID lb/fluid nevery LBtype viscosity density keyword values ...
```

- ID, group-ID are documented in *fix* command
- lb/fluid = style name of this fix command
- nevery = update the lattice-Boltzmann fluid every this many timesteps
- LBtype = 1 to use the standard finite difference LB integrator, 2 to use the LB integrator of *Ollila et al.*
- viscosity = the fluid viscosity (units of mass/(time*length)).
- density = the fluid density.
- zero or more keyword/value pairs may be appended
- keyword = *setArea* or *setGamma* or *scaleGamma* or *dx* or *dm* or *a0* or *noise* or *calcforce* or *trilinear* or *D3Q19* or *read_restart* or *write_restart* or *zwall_velocity* or *bodyforce* or *printfluid*

```
setArea values = type node_area
    type = atom type (1-N)
    node_area = portion of the surface area of the composite object␣
↪associated with the particular atom type (used when the force coupling␣
↪constant is set by default).
setGamma values = gamma
    gamma = user set value for the force coupling constant.
scaleGamma values = type gammaFactor
    type = atom type (1-N)
    gammaFactor = factor to scale the setGamma gamma value by, for the␣
↪specified atom type.
dx values = dx_LB = the lattice spacing.
```

```
dm values = dm_LB = the lattice-Boltzmann mass unit.
a0 values = a_0_real = the square of the speed of sound in the fluid.
noise values = Temperature seed
    Temperature = fluid temperature.
    seed = random number generator seed (positive integer)
calcforce values = N forcegroup-ID
    N = output the force and torque every N timesteps
    forcegroup-ID = ID of the particle group to calculate the force and␣
↪torque of
trilinear values = none (used to switch from the default Peskin␣
↪interpolation stencil to the trilinear stencil).
D3Q19 values = none (used to switch from the default D3Q15, 15 velocity␣
↪lattice, to the D3Q19, 19 velocity lattice).
read_restart values = restart file = name of the restart file to use to␣
↪restart a fluid run.
write_restart values = N = write a restart file every N MD timesteps.
zwall_velocity values = velocity_bottom velocity_top = velocities along␣
↪the y-direction of the bottom and top walls (located at z=zmin and␣
↪z=zmax).
bodyforce values = bodyforcex bodyforcey bodyforcez = the x,y and z␣
↪components of a constant body force added to the fluid.
printfluid values = N = print the fluid density and velocity at each grid␣
↪point every N timesteps.
```

16.75.2 Examples

```
fix 1 all lb/fluid 1 2 1.0 1.0 setGamma 13.0 dx 4.0 dm 10.0 calcforce sphere1
fix 1 all lb/fluid 1 1 1.0 0.0009982071 setArea 1 1.144592082 dx 2.0 dm 0.3 trilinear␣
↪noise 300.0 8979873
```

16.75.3 Description

Implement a lattice-Boltzmann fluid on a uniform mesh covering the LAMMPS simulation domain. The MD particles described by *group-ID* apply a velocity dependent force to the fluid.

The lattice-Boltzmann algorithm solves for the fluid motion governed by the Navier Stokes equations,

$$\begin{aligned}\partial_t \rho + \partial_\beta \left(\rho u_\beta\right) =& 0 \\ \partial_t \left(\rho u_\alpha\right) + \partial_\beta \left(\rho u_\alpha u_\beta\right) =& \partial_\beta \sigma_{\alpha\beta} + F_\alpha + \partial_\beta \left(\eta_{\alpha\beta\gamma\nu} \partial_\gamma u_\nu\right)\end{aligned}$$

with,

$$\eta_{\alpha\beta\gamma\nu} = \eta \left[\delta_{\alpha\gamma}\delta_{\beta\nu} + \delta_{\alpha\nu}\delta_{\beta\gamma} - \frac{2}{3}\delta_{\alpha\beta}\delta_{\gamma\nu}\right] + \Lambda \delta_{\alpha\beta}\delta_{\gamma\nu}$$

where ρ is the fluid density, u is the local fluid velocity, σ is the stress tensor, F is a local external force, and η and Λ are the shear and bulk viscosities respectively. Here, we have implemented

$$\sigma_{\alpha\beta} = -P_{\alpha\beta} = -\rho a_0 \delta_{\alpha\beta}$$

with a_0 set to $\frac{1}{3}\frac{dx}{dt}^2$ by default.

The algorithm involves tracking the time evolution of a set of partial distribution functions which evolve according to a velocity discretized version of the Boltzmann equation,

$$(\partial_t + e_{i\alpha}\partial_\alpha) f_i = -\frac{1}{\tau}(f_i - f_i^{eq}) + W_i$$

where the first term on the right hand side represents a single time relaxation towards the equilibrium distribution function, and τ is a parameter physically related to the viscosity. On a technical note, we have implemented a 15 velocity model (D3Q15) as default; however, the user can switch to a 19 velocity model (D3Q19) through the use of the *D3Q19* keyword. This fix provides the user with the choice of two algorithms to solve this equation, through the specification of the keyword *LBtype*. If *LBtype* is set equal to 1, the standard finite difference LB integrator is used. If *LBtype* is set equal to 2, the algorithm of *Ollila et al.* is used.

Physical variables are then defined in terms of moments of the distribution functions,

$$\rho = \sum_i f_i$$
$$\rho u_\alpha = \sum_i f_i e_{i\alpha}$$

Full details of the lattice-Boltzmann algorithm used can be found in *Mackay et al.*.

The fluid is coupled to the MD particles described by *group-ID* through a velocity dependent force. The contribution to the fluid force on a given lattice mesh site j due to MD particle α is calculated as:

$$\mathbf{F}_{j\alpha} = \gamma(\mathbf{v}_n - \mathbf{u}_f)\zeta_{j\alpha}$$

where $\mathbf{v}_n$ is the velocity of the MD particle, $\mathbf{u}_f$ is the fluid velocity interpolated to the particle location, and γ is the force coupling constant. ζ is a weight assigned to the grid point, obtained by distributing the particle to the nearest lattice sites. For this, the user has the choice between a trilinear stencil, which provides a support of 8 lattice sites, or the immersed boundary method Peskin stencil, which provides a support of 64 lattice sites. While the Peskin stencil is seen to provide more stable results, the trilinear stencil may be better suited for simulation of objects close to walls, due to its smaller support. Therefore, by default, the Peskin stencil is used; however the user may switch to the trilinear stencil by specifying the keyword, *trilinear*.

By default, the force coupling constant, γ, is calculated according to

$$\gamma = \frac{2m_u m_v}{m_u + m_v}\left(\frac{1}{\Delta t_{collision}}\right)$$

Here, m_v is the mass of the MD particle, m_u is a representative fluid mass at the particle location, and $\Delta t_{collision}$ is a collision time, chosen such that $\frac{\tau}{\Delta t_{collision}} = 1$ (see *Mackay and Denniston* for full details). In order to calculate m_u, the fluid density is interpolated to the MD particle location, and multiplied by a volume, node_area * dx_{LB}, where node_area represents the portion of the surface area of the composite object associated with a given MD particle. By default, node_area is set equal to dx_{LB}^2; however specific values for given atom types can be set using the *setArea* keyword.

The user also has the option of specifying their own value for the force coupling constant, for all the MD particles associated with the fix, through the use of the *setGamma* keyword. This may be useful when modelling porous particles. See *Mackay et al.* for a detailed description of the method by which the user can choose an appropriate γ value.

Note: while this fix applies the force of the particles on the fluid, it does not apply the force of the fluid to the particles. When the force coupling constant is set using the default method, there is only one option to include this hydrodynamic force on the particles, and that is through the use of the *lb/viscous* fix. This fix adds the hydrodynamic force to the total force acting on the particles, after which any of the built-in LAMMPS integrators can be used to integrate the particle motion. However, if the user specifies their own value for the force coupling constant, as mentioned in *Mackay et*

al., the built-in LAMMPS integrators may prove to be unstable. Therefore, we have included our own integrators *fix lb/rigid/pc/sphere*, and *fix lb/pc*, to solve for the particle motion in these cases. These integrators should not be used with the *lb/viscous* fix, as they add hydrodynamic forces to the particles directly. In addition, they can not be used if the force coupling constant has been set the default way.

Note: if the force coupling constant is set using the default method, and the *lb/viscous* fix is NOT used to add the hydrodynamic force to the total force acting on the particles, this physically corresponds to a situation in which an infinitely massive particle is moving through the fluid (since collisions between the particle and the fluid do not act to change the particle's velocity). Therefore, the user should set the mass of the particle to be significantly larger than the mass of the fluid at the particle location, in order to approximate an infinitely massive particle (see the dragforce test run for an example).

Inside the fix, parameters are scaled by the lattice-Boltzmann timestep, dt_{LB}, grid spacing, dx_{LB}, and mass unit, dm_{LB}. dt_{LB} is set equal to $\mathrm{nevery} \cdot dt_{MD}$, where dt_{MD} is the MD timestep. By default, dm_{LB} is set equal to 1.0, and dx_{LB} is chosen so that $\frac{\tau}{dt} = \frac{3\eta dt}{\rho dx^2}$ is approximately equal to 1. However, the user has the option of specifying their own values for dm_{LB}, and dx_{LB}, by using the optional keywords *dm*, and *dx* respectively.

Note: Care must be taken when choosing both a value for dx_{LB}, and a simulation domain size. This fix uses the same subdivision of the simulation domain among processors as the main LAMMPS program. In order to uniformly cover the simulation domain with lattice sites, the lengths of the individual LAMMPS sub-domains must all be evenly divisible by dx_{LB}. If the simulation domain size is cubic, with equal lengths in all dimensions, and the default value for dx_{LB} is used, this will automatically be satisfied.

Physical parameters describing the fluid are specified through *viscosity*, *density*, and *a0*. If the force coupling constant is set the default way, the surface area associated with the MD particles is specified using the *setArea* keyword. If the user chooses to specify a value for the force coupling constant, this is set using the *setGamma* keyword. These parameters should all be given in terms of the mass, distance, and time units chosen for the main LAMMPS run, as they are scaled by the LB timestep, lattice spacing, and mass unit, inside the fix.

The *setArea* keyword allows the user to associate a surface area with a given atom type. For example if a spherical composite object of radius R is represented as a spherical shell of N evenly distributed MD particles, all of the same type, the surface area per particle associated with that atom type should be set equal to $\frac{4\pi R^2}{N}$. This keyword should only be used if the force coupling constant, γ, is set the default way.

The *setGamma* keyword allows the user to specify their own value for the force coupling constant, γ, instead of using the default value.

The *scaleGamma* keyword should be used in conjunction with the *setGamma* keyword, when the user wishes to specify different γ values for different atom types. This keyword allows the user to scale the *setGamma* γ value by a factor, gammaFactor, for a given atom type.

The *dx* keyword allows the user to specify a value for the LB grid spacing.

The *dm* keyword allows the user to specify the LB mass unit.

If the *a0* keyword is used, the value specified is used for the square of the speed of sound in the fluid. If this keyword is not present, the speed of sound squared is set equal to $\frac{1}{3}\left(\frac{dx_{LB}}{dt_{LB}}\right)^2$. Setting $a0 > (\frac{dx_{LB}}{dt_{LB}})^2$ is not allowed, as this may lead to instabilities.

If the *noise* keyword is used, followed by a positive temperature value, and a positive integer random number seed, a thermal lattice-Boltzmann algorithm is used. If *LBtype* is set equal to 1 (i.e. the standard LB integrator is chosen), the

thermal LB algorithm of *Adhikari et al.* is used; however if *LBtype* is set equal to 2 both the LB integrator, and thermal LB algorithm described in *Ollila et al.* are used.

If the *calcforce* keyword is used, both the fluid force and torque acting on the specified particle group are printed to the screen every N timesteps.

If the keyword *trilinear* is used, the trilinear stencil is used to interpolate the particle nodes onto the fluid mesh. By default, the immersed boundary method, Peskin stencil is used. Both of these interpolation methods are described in *Mackay et al.*.

If the keyword *D3Q19* is used, the 19 velocity (D3Q19) lattice is used by the lattice-Boltzmann algorithm. By default, the 15 velocity (D3Q15) lattice is used.

If the keyword *write_restart* is used, followed by a positive integer, N, a binary restart file is printed every N LB timesteps. This restart file only contains information about the fluid. Therefore, a LAMMPS restart file should also be written in order to print out full details of the simulation.

Note: When a large number of lattice grid points are used, the restart files may become quite large.

In order to restart the fluid portion of the simulation, the keyword *read_restart* is specified, followed by the name of the binary lb_fluid restart file to be used.

If the *zwall_velocity* keyword is used y-velocities are assigned to the lower and upper walls. This keyword requires the presence of walls in the z-direction. This is set by assigning fixed boundary conditions in the z-direction. If fixed boundary conditions are present in the z-direction, and this keyword is not used, the walls are assumed to be stationary.

If the *bodyforce* keyword is used, a constant body force is added to the fluid, defined by it's x, y and z components.

If the *printfluid* keyword is used, followed by a positive integer, N, the fluid densities and velocities at each lattice site are printed to the screen every N timesteps.

For further details, as well as descriptions and results of several test runs, see *Mackay et al.*. Please include a citation to this paper if the lb_fluid fix is used in work contributing to published research.

Restart, fix_modify, output, run start/stop, minimize info:

Due to the large size of the fluid data, this fix writes it's own binary restart files, if requested, independent of the main LAMMPS *binary restart files*; no information about *lb_fluid* is written to the main LAMMPS *binary restart files*.

None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.75.4 Restrictions

This fix is part of the USER-LB package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix can only be used with an orthogonal simulation domain.

Walls have only been implemented in the z-direction. Therefore, the boundary conditions, as specified via the main LAMMPS boundary command must be periodic for x and y, and either fixed or periodic for z. Shrink-wrapped boundary conditions are not permitted with this fix.

This fix must be used before any of *fix lb/viscous*, *fix lb/momentum*, *fix lb/rigid/pc/sphere*, and/ or *fix lb/pc* , as the fluid needs to be initialized before any of these routines try to access its properties. In addition, in order for the

hydrodynamic forces to be added to the particles, this fix must be used in conjunction with the *lb/viscous* fix if the force coupling constant is set by default, or either the *lb/viscous* fix or one of the *lb/rigid/pc/sphere* or *lb/pc* integrators, if the user chooses to specify their own value for the force coupling constant.

16.75.5 Related commands

fix lb/viscous, *fix lb/momentum*, *fix lb/rigid/pc/sphere*, *fix lb/pc*

16.75.6 Default

By default, the force coupling constant is set according to

$$\gamma = \frac{2m_u m_v}{m_u + m_v}\left(\frac{1}{\Delta t_{collision}}\right)$$

and an area of dx_{LB}^2 per node, used to calculate the fluid mass at the particle node location, is assumed.

dx is chosen such that $\frac{\tau}{dt_{LB}} = \frac{3\eta dt_{LB}}{\rho dx_{LB}^2}$ is approximately equal to 1. *dm* is set equal to 1.0. *a0* is set equal to $\frac{1}{3}\left(\frac{dx_{LB}}{dt_{LB}}\right)^2$. The Peskin stencil is used as the default interpolation method. The D3Q15 lattice is used for the lattice-Boltzmann algorithm. If walls are present, they are assumed to be stationary.

(Ollila et al.) Ollila, S.T.T., Denniston, C., Karttunen, M., and Ala-Nissila, T., Fluctuating lattice-Boltzmann model for complex fluids, J. Chem. Phys. 134 (2011) 064902.

(Mackay et al.) Mackay, F. E., Ollila, S.T.T., and Denniston, C., Hydrodynamic Forces Implemented into LAMMPS through a lattice-Boltzmann fluid, Computer Physics Communications 184 (2013) 2021-2031.

(Mackay and Denniston) Mackay, F. E., and Denniston, C., Coupling MD particles to a lattice-Boltzmann fluid through the use of conservative forces, J. Comput. Phys. 237 (2013) 289-298.

(Adhikari et al.) Adhikari, R., Stratford, K., Cates, M. E., and Wagner, A. J., Fluctuating lattice Boltzmann, Europhys. Lett. 71 (2005) 473-479.

16.76 fix lb/momentum command

16.76.1 Syntax

```
fix ID group-ID lb/momentum nevery keyword values ...
```

- ID, group-ID are documented in the *fix* command
- lb/momentum = style name of this fix command
- nevery = adjust the momentum every this many timesteps
- zero or more keyword/value pairs may be appended
- keyword = *linear*

```
linear values = xflag yflag zflag
  xflag,yflag,zflag = 0/1 to exclude/include each dimension.
```

16.76.2 Examples

```
fix 1 sphere lb/momentum
fix 1 all lb/momentum linear 1 1 0
```

16.76.3 Description

This fix is based on the *fix momentum* command, and was created to be used in place of that command, when a lattice-Boltzmann fluid is present.

Zero the total linear momentum of the system, including both the atoms specified by group-ID and the lattice-Boltzmann fluid every nevery timesteps. This is accomplished by adjusting the particle velocities and the fluid velocities at each lattice site.

Note: This fix only considers the linear momentum of the system.

By default, the subtraction is performed for each dimension. This can be changed by specifying the keyword *linear*, along with a set of three flags set to 0/1 in order to exclude/ include the corresponding dimension.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.76.4 Restrictions

Can only be used if a lattice-Boltzmann fluid has been created via the *fix lb/fluid* command, and must come after this command.

This fix is part of the USER-LB package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.76.5 Related commands

fix momentum, *fix lb/fluid*

16.76.6 Default

Zeros the total system linear momentum in each dimension.

16.77 fix lb/pc command

16.77.1 Syntax

```
fix ID group-ID lb/pc
```

- ID, group-ID are documented in the *fix* command
- lb/pc = style name of this fix command

16.77.2 Examples

```
fix 1 all lb/pc
```

16.77.3 Description

Update the positions and velocities of the individual particles described by *group-ID*, experiencing velocity-dependent hydrodynamic forces, using the integration algorithm described in *Mackay et al.*. This integration algorithm should only be used if a user-specified value for the force-coupling constant used in *fix lb/fluid* has been set; do not use this integration algorithm if the force coupling constant has been set by default.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.77.4 Restrictions

This fix is part of the USER-LB package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Can only be used if a lattice-Boltzmann fluid has been created via the *fix lb/fluid* command, and must come after this command.

16.77.5 Related commands

fix lb/fluid fix lb/rigid/pc/sphere

Default: None.

(Mackay et al.) Mackay, F. E., Ollila, S.T.T., and Denniston, C., Hydrodynamic Forces Implemented into LAMMPS through a lattice-Boltzmann fluid, Computer Physics Communications 184 (2013) 2021-2031.

16.78 fix lb/rigid/pc/sphere command

16.78.1 Syntax

```
fix ID group-ID lb/rigid/pc/sphere bodystyle args keyword values ...
```

- ID, group-ID are documented in *fix* command
- lb/rigid/pc/sphere = style name of this fix command
- bodystyle = *single* or *molecule* or *group*

```
single args = none
molecule args = none
group args = N groupID1 groupID2 ...
  N = # of groups
```

- zero or more keyword/value pairs may be appended
- keyword = *force* or *torque* or *innerNodes*

```
force values = M xflag yflag zflag
  M = which rigid body from 1-Nbody (see asterisk form below)
  xflag,yflag,zflag = off/on if component of center-of-mass force is␣
↪active
torque values = M xflag yflag zflag
  M = which rigid body from 1-Nbody (see asterisk form below)
  xflag,yflag,zflag = off/on if component of center-of-mass torque is␣
↪active
innerNodes values = innergroup-ID
  innergroup-ID = ID of the atom group which does not experience a␣
↪hydrodynamic force from the lattice-Boltzmann fluid
```

16.78.2 Examples

```
fix 1 spheres lb/rigid/pc/sphere
fix 1 all lb/rigid/pc/sphere force 1 0 0 innerNodes ForceAtoms
```

16.78.3 Description

This fix is based on the *fix rigid* command, and was created to be used in place of that fix, to integrate the equations of motion of spherical rigid bodies when a lattice-Boltzmann fluid is present with a user-specified value of the force-coupling constant. The fix uses the integration algorithm described in *Mackay et al.* to update the positions, velocities, and orientations of a set of spherical rigid bodies experiencing velocity dependent hydrodynamic forces. The spherical bodies are assumed to rotate as solid, uniform density spheres, with moments of inertia calculated using the combined sum of the masses of all the constituent particles (which are assumed to be point particles).

By default, all of the atoms that this fix acts on experience a hydrodynamic force due to the presence of the lattice-Boltzmann fluid. However, the *innerNodes* keyword allows the user to specify atoms belonging to a rigid object which do not interact with the lattice-Boltzmann fluid (i.e. these atoms do not feel a hydrodynamic force from the lattice-Boltzmann fluid). This can be used to distinguish between atoms on the surface of a non-porous object, and those on the inside.

This feature can be used, for example, when implementing a hard sphere interaction between two spherical objects. Instead of interactions occurring between the particles on the surfaces of the two spheres, it is desirable simply to place an atom at the center of each sphere, which does not contribute to the hydrodynamic force, and have these central atoms interact with one another.

Apart from the features described above, this fix is very similar to the rigid fix (although it includes fewer optional arguments, and assumes the constituent atoms are point particles); see *fix rigid* for a complete documentation.

Restart, fix_modify, output, run start/stop, minimize info:

No information about the *rigid* and *rigid/nve* fixes are written to *binary restart files*.

Similar to the *fix rigid* command: The rigid fix computes a global scalar which can be accessed by various *output commands*. The scalar value calculated by these fixes is "intensive". The scalar is the current temperature of the collection of rigid bodies. This is averaged over all rigid bodies and their translational and rotational degrees of freedom. The translational energy of a rigid body is 1/2 m v^2, where m = total mass of the body and v = the velocity of its center of mass. The rotational energy of a rigid body is 1/2 I w^2, where I = the moment of inertia tensor of the body and w = its angular velocity. Degrees of freedom constrained by the *force* and *torque* keywords are removed from this calculation.

All of these fixes compute a global array of values which can be accessed by various *output commands*. The number of rows in the array is equal to the number of rigid bodies. The number of columns is 15. Thus for each rigid body, 15 values are stored: the xyz coords of the center of mass (COM), the xyz components of the COM velocity, the xyz components of the force acting on the COM, the xyz components of the torque acting on the COM, and the xyz image flags of the COM, which have the same meaning as image flags for atom positions (see the "dump" command). The force and torque values in the array are not affected by the *force* and *torque* keywords in the fix rigid command; they reflect values before any changes are made by those keywords.

The ordering of the rigid bodies (by row in the array) is as follows. For the *single* keyword there is just one rigid body. For the *molecule* keyword, the bodies are ordered by ascending molecule ID. For the *group* keyword, the list of group IDs determines the ordering of bodies.

The array values calculated by these fixes are "intensive", meaning they are independent of the number of atoms in the simulation.

No parameter of these fixes can be used with the *start/stop* keywords of the *run* command. These fixes are not invoked during *energy minimization*.

16.78.4 Restrictions

This fix is part of the USER-LB package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Can only be used if a lattice-Boltzmann fluid has been created via the *fix lb/fluid* command, and must come after this command. Should only be used if the force coupling constant used in *fix lb/fluid* has been set by the user; this integration fix cannot be used if the force coupling constant is set by default.

16.78.5 Related commands

fix lb/fluid, *fix lb/pc*

16.78.6 Default

The defaults are force * on on on, and torque * on on on.

(Mackay et al.) Mackay, F. E., Ollila, S.T.T., and Denniston, C., Hydrodynamic Forces Implemented into LAMMPS through a lattice-Boltzmann fluid, Computer Physics Communications 184 (2013) 2021-2031.

16.79 fix lb/viscous command

16.79.1 Syntax

```
fix ID group-ID lb/viscous
```

- ID, group-ID are documented in *fix* command
- lb/viscous = style name of this fix command

16.79.2 Examples

fix 1 flow lb/viscous

16.79.3 Description

This fix is similar to the *fix viscous* command, and is to be used in place of that command when a lattice-Boltzmann fluid is present, and the user wishes to integrate the particle motion using one of the built in LAMMPS integrators.

This fix adds a force, F = - Gamma*(velocity-fluid_velocity), to each atom, where Gamma is the force coupling constant described in the *fix lb/fluid* command (which applies an equal and opposite force to the fluid).

Note: This fix should only be used in conjunction with one of the built in LAMMPS integrators; it should not be used with the *fix lb/pc* or *fix lb/rigid/pc/sphere* integrators, which already include the hydrodynamic forces. These latter fixes should only be used if the force coupling constant has been set by the user (instead of using the default value); if the default force coupling value is used, then this fix provides the only method for adding the hydrodynamic forces to the particles.

For further details, as well as descriptions and results of several test runs, see *Mackay et al.*. Please include a citation to this paper if this fix is used in work contributing to published research.

Restart, fix_modify, output, run start/stop, minimize info:

As described in the *fix viscous* documentation:

"No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command. This fix should only be used with damped dynamics minimizers that allow for non-conservative forces. See the *min_style* command for details."

16.79.4 Restrictions

This fix is part of the USER-LB package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Can only be used if a lattice-Boltzmann fluid has been created via the *fix lb/fluid* command, and must come after this command.

This fix should not be used if either the *fix lb/pc* or *fix lb/rigid/pc/sphere* integrator is used.

16.79.5 Related commands

fix lb/fluid, *fix lb/pc*, *fix lb/rigid/pc/sphere*

Default: none

(Mackay et al.) Mackay, F. E., Ollila, S.T.T., and Denniston, C., Hydrodynamic Forces Implemented into LAMMPS through a lattice-Boltzmann fluid, Computer Physics Communications 184 (2013) 2021-2031.

16.80 fix lineforce command

16.80.1 Syntax

```
fix ID group-ID lineforce x y z
```

- ID, group-ID are documented in *fix* command
- lineforce = style name of this fix command
- x y z = direction of line as a 3-vector

16.80.2 Examples

```
fix hold boundary lineforce 0.0 1.0 1.0
```

16.80.3 Description

Adjust the forces on each atom in the group so that only the component of force along the linear direction specified by the vector (x,y,z) remains. This is done by subtracting out components of force in the plane perpendicular to the line.

If the initial velocity of the atom is 0.0 (or along the line), then it should continue to move along the line thereafter.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command.

16.80.4 Restrictions

none

16.80.5 Related commands

fix planeforce

Default: none

16.81 fix manifoldforce command

16.81.1 Syntax

```
fix ID group-ID manifoldforce manifold manifold-args ...
```

- ID, group-ID are documented in *fix* command
- manifold = name of the manifold
- manifold-args = parameters for the manifold

16.81.2 Examples

fix constrain all manifoldforce sphere 5.0

16.81.3 Description

This fix subtracts each time step from the force the component along the normal of the specified *manifold*. This can be used in combination with *minimize* to remove overlap between particles while keeping them (roughly) constrained to the given manifold, e.g. to set up a run with *fix nve/manifold/rattle*. I have found that only *hftn* and *quickmin* with a very small time step perform adequately though.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is invoked during *energy minimization*.

16.81.4 Restrictions

This fix is part of the USER-MANIFOLD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Only use this with *min_style hftn* or *min_style quickmin*. If not, the constraints will not be satisfied very well at all. A warning is generated if the *min_style* is incompatible but no error.

16.81.5 Related commands

fix nve/manifold/rattle, *fix nvt/manifold/rattle*

16.82 fix meso command

16.82.1 Syntax

```
fix ID group-ID meso
```

- ID, group-ID are documented in *fix* command
- meso = style name of this fix command

16.82.2 Examples

```
fix 1 all meso
```

16.82.3 Description

Perform time integration to update position, velocity, internal energy and local density for atoms in the group each timestep. This fix is needed to time-integrate mesoscopic systems where particles carry internal variables such as SPH or DPDE.

See this PDF guide to using SPH in LAMMPS.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.82.4 Restrictions

This fix is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.82.5 Related commands

"fix meso/stationary"

Default: none

16.83 fix meso/move command

16.83.1 Syntax

```
fix ID group-ID meso/move style args keyword values ...
```

- ID, group-ID are documented in *fix* command
- meso/move = style name of this fix command
- style = *linear* or *wiggle* or *rotate* or *variable*

```
linear args = Vx Vy Vz
  Vx,Vy,Vz = components of velocity vector (velocity units), any␣
↪component can be specified as NULL
wiggle args = Ax Ay Az period
  Ax,Ay,Az = components of amplitude vector (distance units), any␣
↪component can be specified as NULL
  period = period of oscillation (time units)
rotate args = Px Py Pz Rx Ry Rz period
  Px,Py,Pz = origin point of axis of rotation (distance units)
  Rx,Ry,Rz = axis of rotation vector
  period = period of rotation (time units)
variable args = v_dx v_dy v_dz v_vx v_vy v_vz
  v_dx,v_dy,v_dz = 3 variable names that calculate x,y,z displacement as␣
↪function of time, any component can be specified as NULL
  v_vx,v_vy,v_vz = 3 variable names that calculate x,y,z velocity as␣
↪function of time, any component can be specified as NULL
```

- zero or more keyword/value pairs may be appended
- keyword = *units*

```
units value = box or lattice
```

16.83.2 Examples

```
fix 1 boundary meso/move wiggle 3.0 0.0 0.0 1.0 units box
fix 2 boundary meso/move rotate 0.0 0.0 0.0 0.0 0.0 1.0 5.0
fix 2 boundary meso/move variable v_myx v_myy NULL v_VX v_VY NULL
```

16.83.3 Description

Perform updates of position, velocity, internal energy and local density for mesoscopic particles in the group each timestep using the specified settings or formulas, without regard to forces on the particles. This can be useful for boundary, solid bodies or other particles, whose movement can influence nearby particles.

The operation of this fix is exactly like that described by the *fix move* command, except that particles' density, internal energy and extrapolated velocity are also updated.

Note: The particles affected by this fix should not be time integrated by other fixes (e.g. *fix meso*, *fix meso/stationary*), since that will change their positions and velocities twice.

Note: As particles move due to this fix, they will pass through periodic boundaries and be remapped to the other side of the simulation box, just as they would during normal time integration (e.g. via the *fix meso* command). It is up to you to decide whether periodic boundaries are appropriate with the kind of particle motion you are prescribing with this fix.

Note: As discussed below, particles are moved relative to their initial position at the time the fix is specified. These initial coordinates are stored by the fix in "unwrapped" form, by using the image flags associated with each particle. See the *dump custom* command for a discussion of "unwrapped" coordinates. See the Atoms section of the *read_data* command for a discussion of image flags and how they are set for each particle. You can reset the image flags (e.g. to 0) before invoking this fix by using the *set image* command.

The *linear* style moves particles at a constant velocity, so that their position X = (x,y,z) as a function of time is given in vector notation as

```
X(t) = X0 + V * delta
```

where *X0* = (x0,y0,z0) is their position at the time the fix is specified, *V* is the specified velocity vector with components (Vx,Vy,Vz), and *delta* is the time elapsed since the fix was specified. This style also sets the velocity of each particle to V = (Vx,Vy,Vz). If any of the velocity components is specified as NULL, then the position and velocity of that component is time integrated the same as the *fix meso* command would perform, using the corresponding force component on the particle.

Note that the *linear* style is identical to using the *variable* style with an *equal-style variable* that uses the vdisplace() function. E.g.

```
variable V equal 10.0
variable x equal vdisplace(0.0,$V)
fix 1 boundary move variable v_x NULL NULL v_V NULL NULL
```

The *wiggle* style moves particles in an oscillatory fashion, so that their position X = (x,y,z) as a function of time is given in vector notation as

```
X(t) = X0 + A sin(omega*delta)
```

where *X0* = (x0,y0,z0) is their position at the time the fix is specified, *A* is the specified amplitude vector with components (Ax,Ay,Az), *omega* is 2 PI / *period*, and *delta* is the time elapsed since the fix was specified. This style also sets the velocity of each particle to the time derivative of this expression. If any of the amplitude components is specified as NULL, then the position and velocity of that component is time integrated the same as the *fix meso* command would perform, using the corresponding force component on the particle.

Note that the *wiggle* style is identical to using the *variable* style with *equal-style variables* that use the swiggle() and cwiggle() functions. E.g.

```
variable A equal 10.0
variable T equal 5.0
variable omega equal 2.0*PI/$T
variable x equal swiggle(0.0,$A,$T)
variable v equal v_omega*($A-cwiggle(0.0,$A,$T))
fix 1 boundary move variable v_x NULL NULL v_v NULL NULL
```

The *rotate* style rotates particles around a rotation axis *R* = (Rx,Ry,Rz) that goes through a point *P* = (Px,Py,Pz). The *period* of the rotation is also specified. The direction of rotation for the particles around the rotation axis is consistent with the right-hand rule: if your right-hand thumb points along *R*, then your fingers wrap around the axis in the direction of rotation.

This style also sets the velocity of each particle to (omega cross Rperp) where omega is its angular velocity around the rotation axis and Rperp is a perpendicular vector from the rotation axis to the particle.

The *variable* style allows the position and velocity components of each particle to be set by formulas specified via the *variable* command. Each of the 6 variables is specified as an argument to the fix as v_name, where name is the variable name that is defined elsewhere in the input script.

Each variable must be of either the *equal* or *atom* style. *Equal*-style variables compute a single numeric quantity, that can be a function of the timestep as well as of other simulation values. *Atom*-style variables compute a numeric quantity for each particle, that can be a function per-atom quantities, such as the particle's position, as well as of the timestep and other simulation values. Note that this fix stores the original coordinates of each particle (see note below) so that per-atom quantity can be used in an atom-style variable formula. See the *variable* command for details.

The first 3 variables (v_dx,v_dy,v_dz) specified for the *variable* style are used to calculate a displacement from the particle's original position at the time the fix was specified. The second 3 variables (v_vx,v_vy,v_vz) specified are used to compute a velocity for each particle.

Any of the 6 variables can be specified as NULL. If both the displacement and velocity variables for a particular x,y,z component are specified as NULL, then the position and velocity of that component is time integrated the same as the *fix meso* command would perform, using the corresponding force component on the particle. If only the velocity variable for a component is specified as NULL, then the displacement variable will be used to set the position of the particle, and its velocity component will not be changed. If only the displacement variable for a component is specified as NULL, then the velocity variable will be used to set the velocity of the particle, and the position of the particle will be time integrated using that velocity.

The *units* keyword determines the meaning of the distance units used to define the *linear* velocity and *wiggle* amplitude and *rotate* origin. This setting is ignored for the *variable* style. A *box* value selects standard units as defined by the *units* command, e.g. velocity in Angstroms/fmsec and amplitude and position in Angstroms for units = real. A *lattice* value means the velocity units are in lattice spacings per time and the amplitude and position are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacing. Each of these 3 quantities may be dependent on the x,y,z dimension, since the lattice spacings can be different in x,y,z.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the original coordinates of moving particles to *binary restart files*, as well as the initial timestep, so that the motion can be continuous in a restarted simulation. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

Note: Because the move positions are a function of the current timestep and the initial timestep, you cannot reset the timestep to a different value after reading a restart file, if you expect a fix move command to work in an uninterrupted fashion.

None of the *fix_modify* options are relevant to this fix.

This fix produces a per-atom array which can be accessed by various *output commands*. The number of columns for each atom is 3, and the columns store the original unwrapped x,y,z coords of each particle. The per-atom values can be accessed on any timestep.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

This fix is not invoked during *energy minimization*.

16.83.4 Restrictions

This fix is part of the USER-SDPD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix requires that atoms store density and internal energy as defined by the *atom_style meso* command.

All particles in the group must be mesoscopic SPH/SDPD particles.

16.83.5 Related commands

fix move, *fix meso*, *displace_atoms*

16.83.6 Default

The option default is units = lattice.

16.84 fix meso/stationary command

16.84.1 Syntax

```
fix ID group-ID meso/stationary
```

- ID, group-ID are documented in *fix* command
- meso = style name of this fix command

16.84.2 Examples

```
fix 1 boundary meso/stationary
```

16.84.3 Description

Perform time integration to update internal energy and local density, but not position or velocity for atoms in the group each timestep. This fix is needed for SPH simulations to correctly time-integrate fixed boundary particles which constrain a fluid to a given region in space.

See this PDF guide to using SPH in LAMMPS.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.84.4 Restrictions

This fix is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.84.5 Related commands

"fix meso"

Default: none

16.85 fix momentum command

16.86 fix momentum/kk command

16.86.1 Syntax

```
fix ID group-ID momentum N keyword values ...
```

- ID, group-ID are documented in *fix* command
- momentum = style name of this fix command
- N = adjust the momentum every this many timesteps one or more keyword/value pairs may be appended
- keyword = *linear* or *angular* or *rescale*

```
linear values = xflag yflag zflag
  xflag,yflag,zflag = 0/1 to exclude/include each dimension
angular values = none
```

```
rescale values = none
```

16.86.2 Examples

```
fix 1 all momentum 1 linear 1 1 0
fix 1 all momentum 1 linear 1 1 1 rescale
fix 1 all momentum 100 linear 1 1 1 angular
```

16.86.3 Description

Zero the linear and/or angular momentum of the group of atoms every N timesteps by adjusting the velocities of the atoms. One (or both) of the *linear* or *angular* keywords must be specified.

If the *linear* keyword is used, the linear momentum is zeroed by subtracting the center-of-mass velocity of the group from each atom. This does not change the relative velocity of any pair of atoms. One or more dimensions can be excluded from this operation by setting the corresponding flag to 0.

If the *angular* keyword is used, the angular momentum is zeroed by subtracting a rotational component from each atom.

This command can be used to insure the entire collection of atoms (or a subset of them) does not drift or rotate during the simulation due to random perturbations (e.g. *fix langevin* thermostatting).

The *rescale* keyword enables conserving the kinetic energy of the group of atoms by rescaling the velocities after the momentum was removed.

Note that the *velocity* command can be used to create initial velocities with zero aggregate linear and/or angular momentum.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.86.4 Restrictions

none

16.86.5 Related commands

fix recenter, *velocity*

Default: none

16.87 fix move command

16.87.1 Syntax

```
fix ID group-ID move style args keyword values ...
```

- ID, group-ID are documented in *fix* command
- move = style name of this fix command
- style = *linear* or *wiggle* or *rotate* or *variable*

```
linear args = Vx Vy Vz
  Vx,Vy,Vz = components of velocity vector (velocity units), any␣
↪component can be specified as NULL
wiggle args = Ax Ay Az period
  Ax,Ay,Az = components of amplitude vector (distance units), any␣
↪component can be specified as NULL
  period = period of oscillation (time units)
rotate args = Px Py Pz Rx Ry Rz period
  Px,Py,Pz = origin point of axis of rotation (distance units)
  Rx,Ry,Rz = axis of rotation vector
  period = period of rotation (time units)
variable args = v_dx v_dy v_dz v_vx v_vy v_vz
  v_dx,v_dy,v_dz = 3 variable names that calculate x,y,z displacement as␣
↪function of time, any component can be specified as NULL
  v_vx,v_vy,v_vz = 3 variable names that calculate x,y,z velocity as␣
↪function of time, any component can be specified as NULL
```

- zero or more keyword/value pairs may be appended
- keyword = *units*

```
units value = box or lattice
```

16.87.2 Examples

```
fix 1 boundary move wiggle 3.0 0.0 0.0 1.0 units box
fix 2 boundary move rotate 0.0 0.0 0.0 0.0 0.0 1.0 5.0
fix 2 boundary move variable v_myx v_myy NULL v_VX v_VY NULL
```

16.87.3 Description

Perform updates of position and velocity for atoms in the group each timestep using the specified settings or formulas, without regard to forces on the atoms. This can be useful for boundary or other atoms, whose movement can influence nearby atoms.

Note: The atoms affected by this fix should not normally be time integrated by other fixes (e.g. *fix nve*, *fix nvt*), since that will change their positions and velocities twice.

Note: As atoms move due to this fix, they will pass through periodic boundaries and be remapped to the other side of the simulation box, just as they would during normal time integration (e.g. via the *fix nve* command). It is up to you to decide whether periodic boundaries are appropriate with the kind of atom motion you are prescribing with this fix.

Note: As discussed below, atoms are moved relative to their initial position at the time the fix is specified. These initial coordinates are stored by the fix in "unwrapped" form, by using the image flags associated with each atom. See the *dump custom* command for a discussion of "unwrapped" coordinates. See the Atoms section of the *read_data* command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this fix by using the *set image* command.

The *linear* style moves atoms at a constant velocity, so that their position *X* = (x,y,z) as a function of time is given in vector notation as

```
X(t) = X0 + V * delta
```

where *X0* = (x0,y0,z0) is their position at the time the fix is specified, *V* is the specified velocity vector with components (Vx,Vy,Vz), and *delta* is the time elapsed since the fix was specified. This style also sets the velocity of each atom to V = (Vx,Vy,Vz). If any of the velocity components is specified as NULL, then the position and velocity of that component is time integrated the same as the *fix nve* command would perform, using the corresponding force component on the atom.

Note that the *linear* style is identical to using the *variable* style with an *equal-style variable* that uses the vdisplace() function. E.g.

```
variable V equal 10.0
variable x equal vdisplace(0.0,$V)
fix 1 boundary move variable v_x NULL NULL v_V NULL NULL
```

The *wiggle* style moves atoms in an oscillatory fashion, so that their position *X* = (x,y,z) as a function of time is given in vector notation as

```
X(t) = X0 + A sin(omega*delta)
```

where *X0* = (x0,y0,z0) is their position at the time the fix is specified, *A* is the specified amplitude vector with components (Ax,Ay,Az), *omega* is 2 PI / *period*, and *delta* is the time elapsed since the fix was specified. This style also sets the velocity of each atom to the time derivative of this expression. If any of the amplitude components is specified as NULL, then the position and velocity of that component is time integrated the same as the *fix nve* command would perform, using the corresponding force component on the atom.

Note that the *wiggle* style is identical to using the *variable* style with *equal-style variables* that use the swiggle() and cwiggle() functions. E.g.

```
variable A equal 10.0
variable T equal 5.0
variable omega equal 2.0*PI/$T
variable x equal swiggle(0.0,$A,$T)
variable v equal v_omega*($A-cwiggle(0.0,$A,$T))
fix 1 boundary move variable v_x NULL NULL v_v NULL NULL
```

The *rotate* style rotates atoms around a rotation axis *R* = (Rx,Ry,Rz) that goes through a point *P* = (Px,Py,Pz). The *period* of the rotation is also specified. The direction of rotation for the atoms around the rotation axis is consistent with the right-hand rule: if your right-hand thumb points along *R*, then your fingers wrap around the axis in the direction of rotation.

This style also sets the velocity of each atom to (omega cross Rperp) where omega is its angular velocity around the rotation axis and Rperp is a perpendicular vector from the rotation axis to the atom. If the defined *atom_style* assigns an angular velocity or angular momentum or orientation to each atom (*atom styles* sphere, ellipsoid, line, tri, body), then those properties are also updated appropriately to correspond to the atom's motion and rotation over time.

The *variable* style allows the position and velocity components of each atom to be set by formulas specified via the *variable* command. Each of the 6 variables is specified as an argument to the fix as v_name, where name is the variable name that is defined elsewhere in the input script.

Each variable must be of either the *equal* or *atom* style. *Equal*-style variables compute a single numeric quantity, that can be a function of the timestep as well as of other simulation values. *Atom*-style variables compute a numeric quantity for each atom, that can be a function per-atom quantities, such as the atom's position, as well as of the timestep and other simulation values. Note that this fix stores the original coordinates of each atom (see note below) so that per-atom quantity can be used in an atom-style variable formula. See the *variable* command for details.

The first 3 variables (v_dx,v_dy,v_dz) specified for the *variable* style are used to calculate a displacement from the atom's original position at the time the fix was specified. The second 3 variables (v_vx,v_vy,v_vz) specified are used to compute a velocity for each atom.

Any of the 6 variables can be specified as NULL. If both the displacement and velocity variables for a particular x,y,z component are specified as NULL, then the position and velocity of that component is time integrated the same as the *fix nve* command would perform, using the corresponding force component on the atom. If only the velocity variable for a component is specified as NULL, then the displacement variable will be used to set the position of the atom, and its velocity component will not be changed. If only the displacement variable for a component is specified as NULL, then the velocity variable will be used to set the velocity of the atom, and the position of the atom will be time integrated using that velocity.

The *units* keyword determines the meaning of the distance units used to define the *linear* velocity and *wiggle* amplitude and *rotate* origin. This setting is ignored for the *variable* style. A *box* value selects standard units as defined by the *units* command, e.g. velocity in Angstroms/fmsec and amplitude and position in Angstroms for units = real. A *lattice* value means the velocity units are in lattice spacings per time and the amplitude and position are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacing. Each of these 3 quantities may be dependent on the x,y,z dimension, since the lattice spacings can be different in x,y,z.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the original coordinates of moving atoms to *binary restart files*, as well as the initial timestep, so that the motion can be continuous in a restarted simulation. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

Note: Because the move positions are a function of the current timestep and the initial timestep, you cannot reset the timestep to a different value after reading a restart file, if you expect a fix move command to work in an uninterrupted fashion.

None of the *fix_modify* options are relevant to this fix.

This fix produces a per-atom array which can be accessed by various *output commands*. The number of columns for each atom is 3, and the columns store the original unwrapped x,y,z coords of each atom. The per-atom values can be accessed on any timestep.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

For *rRESPA time integration*, this fix adjusts the position and velocity of atoms on the outermost rRESPA level.

16.87.4 Restrictions

none

16.87.5 Related commands

fix nve, *displace_atoms*

Default: none

The option default is units = lattice.

16.88 fix mscg command

16.88.1 Syntax

```
fix ID group-ID mscg N keyword args ...
```

- ID, group-ID are documented in *fix* command
- mscg = style name of this fix command
- N = envoke this fix every this many timesteps
- zero or more keyword/value pairs may be appended
- keyword = *range* or *name* or *max*

```
range arg = on or off
  on = range finding functionality is performed
  off = force matching functionality is performed
name args = name1 ... nameN
  name1,...,nameN = string names for each atom type (1-Ntype)
max args = maxb maxa maxd
  maxb,maxa,maxd = maximum bonds/angles/dihedrals per atom
```

16.88.2 Examples

```
fix 1 all mscg 1
fix 1 all mscg 1 range name A B
fix 1 all mscg 1 max 4 8 20
```

16.88.3 Description

This fix applies the Multi-Scale Coarse-Graining (MSCG) method to snapshots from a dump file to generate potentials for coarse-grained simulations from all-atom simulations, using a force-matching technique (*Izvekov*, *Noid*).

It makes use of the MS-CG library, written and maintained by Greg Voth's group at the University of Chicago, which is freely available on their MS-CG GitHub site. See instructions on obtaining and installing the MS-CG library in the src/MSCG/README file, which must be done before you build LAMMPS with this fix command and use the command in a LAMMPS input script.

An example script using this fix is provided the examples/mscg directory.

The general workflow for using LAMMPS in conjunction with the MS-CG library to create a coarse-grained model and run coarse-grained simulations is as follows:

1. Perform all-atom simulations on the system to be coarse grained.
2. Generate a trajectory mapped to the coarse-grained model.
3. Create input files for the MS-CG library.
4. Run the range finder functionality of the MS-CG library.
5. Run the force matching functionality of the MS-CG library.
6. Check the results of the force matching.
7. Run coarse-grained simulations using the new coarse-grained potentials.

This fix can perform the range finding and force matching steps 4 and 5 of the above workflow when used in conjunction with the *rerun* command. It does not perform steps 1-3 and 6-7.

Step 2 can be performed using a Python script (what is the name?) provided with the MS-CG library which defines the coarse-grained model and converts a standard LAMMPS dump file for an all-atom simulation (step 1) into a LAMMPS dump file which has the positions of and forces on the coarse-grained beads.

In step 3, an input file named "control.in" is needed by the MS-CG library which sets parameters for the range finding and force matching functionalities. See the examples/mscg/control.in file as an example. And see the documentation provided with the MS-CG library for more info on this file.

When this fix is used to perform steps 4 and 5, the MS-CG library also produces additional output files. The range finder functionality (step 4) outputs files defining pair and bonded interaction ranges. The force matching functionality (step 5) outputs tabulated force files for every interaction in the system. Other diagnostic files can also be output depending on the parameters in the MS-CG library input script. Again, see the documentation provided with the MS-CG library for more info.

The *range* keyword specifies which MS-CG library functionality should be invoked. If *on*, the step 4 range finder functionality is invoked. *off*, the step 5 force matching functionality is invoked.

If the *name* keyword is used, string names are defined to associate with the integer atom types in LAMMPS. *Ntype* names must be provided, one for each atom type (1-Ntype).

The *max* keyword specifies the maximum number of bonds, angles, and dihedrals a bead can have in the coarse-grained model.

16.88.4 Restrictions

This fix is part of the MSCG package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

The MS-CG library uses C++11, which may not be supported by older compilers. The MS-CG library also has some additional numeric library dependencies, which are described in its documentation.

Currently, the MS-CG library is not setup to run in parallel with MPI, so this fix can only be used in a serial LAMMPS build and run on a single processor.

Related commands: none

16.88.5 Default

The default keyword settings are range off, max 4 12 36.

(Izvekov) Izvekov, Voth, J Chem Phys 123, 134105 (2005).

(Noid) Noid, Chu, Ayton, Krishna, Izvekov, Voth, Das, Andersen, J Chem Phys 128, 134105 (2008).

16.89 fix msst command

16.89.1 Syntax

```
fix ID group-ID msst dir shockvel keyword value ...
```

- ID, group-ID are documented in *fix* command
- msst = style name of this fix
- dir = *x* or *y* or *z*
- shockvel = shock velocity (strictly positive, distance/time units)
- zero or more keyword value pairs may be appended
- keyword = *q* or *mu* or *p0* or *v0* or *e0* or *tscale* or *beta* or *dftb*

```
q value = cell mass-like parameter (mass^2/distance^4 units)
mu value = artificial viscosity (mass/length/time units)
p0 value = initial pressure in the shock equations (pressure units)
v0 value = initial simulation cell volume in the shock equations␣
↪(distance^3 units)
e0 value = initial total energy (energy units)
tscale value = reduction in initial temperature (unitless fraction␣
↪between 0.0 and 1.0)
dftb value = yes or no for whether using MSST in conjunction with DFTB+
beta value = scale factor for improved energy conservation
```

16.89.2 Examples

```
fix 1 all msst y 100.0 q 1.0e5 mu 1.0e5
fix 2 all msst z 50.0 q 1.0e4 mu 1.0e4  v0 4.3419e+03 p0 3.7797e+03 e0 -9.72360e+02␣
↪tscale 0.01
fix 1 all msst y 100.0 q 1.0e5 mu 1.0e5 dftb yes beta 0.5
```

16.89.3 Description

This command performs the Multi-Scale Shock Technique (MSST) integration to update positions and velocities each timestep to mimic a compressive shock wave passing over the system. See *(Reed)* for a detailed description of this method. The MSST varies the cell volume and temperature in such a way as to restrain the system to the shock Hugoniot and the Rayleigh line. These restraints correspond to the macroscopic conservation laws dictated by a shock front. *shockvel* determines the steady shock velocity that will be simulated.

To perform a simulation, choose a value of *q* that provides volume compression on the timescale of 100 fs to 1 ps. If the volume is not compressing, either the shock speed is chosen to be below the material sound speed or *p0* has been chosen inaccurately. Volume compression at the start can be sped up by using a non-zero value of *tscale*. Use the smallest value of *tscale* that results in compression.

Under some special high-symmetry conditions, the pressure (volume) and/or temperature of the system may oscillate for many cycles even with an appropriate choice of mass-like parameter *q*. Such oscillations have physical significance in some cases. The optional *mu* keyword adds an artificial viscosity that helps break the system symmetry to equilibrate to the shock Hugoniot and Rayleigh line more rapidly in such cases.

The keyword *tscale* is a factor between 0 and 1 that determines what fraction of thermal kinetic energy is converted to compressive strain kinetic energy at the start of the simulation. Setting this parameter to a non-zero value may assist in compression at the start of simulations where it is slow to occur.

If keywords *e0*, *p0*,or *v0* are not supplied, these quantities will be calculated on the first step, after the energy specified by *tscale* is removed. The value of *e0* is not used in the dynamical equations, but is used in calculating the deviation from the Hugoniot.

The keyword *beta* is a scaling term that can be added to the MSST ionic equations of motion to account for drift in the conserved quantity during long timescale simulations, similar to a Berendsen thermostat. See *(Reed)* and *(Goldman)* for more details. The value of *beta* must be between 0.0 and 1.0 inclusive. A value of 0.0 means no contribution, a value of 1.0 means a full contribution.

Values of shockvel less than a critical value determined by the material response will not have compressive solutions. This will be reflected in lack of significant change of the volume in the MSST.

For all pressure styles, the simulation box stays orthogonal in shape. Parrinello-Rahman boundary conditions (tilted box) are supported by LAMMPS, but are not implemented for MSST.

This fix computes a temperature and pressure and potential energy each timestep. To do this, the fix creates its own computes of style "temp" "pressure", and "pe", as if these commands had been issued:

```
compute fix-ID_MSST_temp all temp
compute fix-ID_MSST_press all pressure fix-ID_MSST_temp

compute fix-ID_MSST_pe all pe
```

See the *compute temp* and *compute pressure* commands for details. Note that the IDs of the new computes are the fix-ID + "_MSST_temp" or "MSST_press" or "_MSST_pe". The group for the new computes is "all".

The *dftb* keyword is to allow this fix to be used when LAMMPS is being driven by DFTB+, a density-functional tight-binding code. If the keyword *dftb* is used with a value of *yes*, then the MSST equations are altered to account for the electron entropy contribution to the Hugonio relations and total energy. See *(Reed2)* and *(Goldman)* for details on this contribution. In this case, you must define a *fix external* command in your input script, which is used to callback to DFTB+ during the LAMMPS timestepping. DFTB+ will communicate its info to LAMMPS via that fix.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of all internal variables to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The progress of the MSST can be monitored by printing the global scalar and global vector quantities computed by the fix.

The scalar is the cumulative energy change due to the fix. This is also the energy added to the potential energy by the *fix_modify energy* command. With this command, the thermo keyword *etotal* prints the conserved quantity of the MSST dynamic equations. This can be used to test if the MD timestep is sufficiently small for accurate integration of the dynamic equations. See also *thermo_style* command.

The global vector contains four values in this order:

[*dhugoniot*, *drayleigh*, *lagrangian_speed*, *lagrangian_position*]

1. *dhugoniot* is the departure from the Hugoniot (temperature units).
2. *drayleigh* is the departure from the Rayleigh line (pressure units).
3. *lagrangian_speed* is the laboratory-frame Lagrangian speed (particle velocity) of the computational cell (velocity units).
4. *lagrangian_position* is the computational cell position in the reference frame moving at the shock speed. This is usually a good estimate of distance of the computational cell behind the shock front.

To print these quantities to the log file with descriptive column headers, the following LAMMPS commands are suggested:

```
fix              msst all msst z
fix_modify       msst energy yes
variable dhug    equal f_msst[1]
variable dray    equal f_msst[2]
variable lgr_vel equal f_msst[3]
variable lgr_pos equal f_msst[4]
thermo_style     custom step temp ke pe lz pzz etotal v_dhug v_dray v_lgr_vel v_lgr_
↪pos f_msst
```

These fixes compute a global scalar and a global vector of 4 quantities, which can be accessed by various *output commands*. The scalar values calculated by this fix are "extensive"; the vector values are "intensive".

16.89.4 Restrictions

This fix style is part of the SHOCK package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

All cell dimensions must be periodic. This fix can not be used with a triclinic cell. The MSST fix has been tested only for the group-ID all.

16.89.5 Related commands

fix nphug, *fix deform*

16.89.6 Default

The keyword defaults are q = 10, mu = 0, tscale = 0.01, dftb = no, beta = 0.0. Note that p0, v0, and e0 are calculated on the first timestep.

(Reed) Reed, Fried, and Joannopoulos, Phys. Rev. Lett., 90, 235503 (2003).

(Reed2) Reed, J. Phys. Chem. C, 116, 2205 (2012).

(Goldman) Goldman, Srinivasan, Hamel, Fried, Gaus, and Elstner, J. Phys. Chem. C, 117, 7885 (2013).

16.90 fix mvv/dpd command

16.91 fix mvv/edpd command

16.92 fix mvv/tdpd command

16.92.1 Syntax

```
fix ID group-ID mvv/dpd lambda

fix ID group-ID mvv/edpd lambda

fix ID group-ID mvv/tdpd lambda
```

- ID, group-ID are documented in *fix* command
- mvv/dpd, mvv/edpd, mvv/tdpd = style name of this fix command
- lambda = (optional) relaxation parameter (unitless)

16.92.2 Examples

```
fix 1 all mvv/dpd
fix 1 all mvv/dpd 0.5
fix 1 all mvv/edpd
fix 1 all mvv/edpd 0.5
fix 1 all mvv/tdpd
fix 1 all mvv/tdpd 0.5
```

16.92.3 Description

Perform time integration using the modified velocity-Verlet (MVV) algorithm to update position and velocity (fix mvv/dpd), or position, velocity and temperature (fix mvv/edpd), or position, velocity and concentration (fix mvv/tdpd) for particles in the group each timestep.

The modified velocity-Verlet (MVV) algorithm aims to improve the stability of the time integrator by using an extrapolated version of the velocity for the force evaluation:

$$
\begin{aligned}
v(t+\frac{\Delta t}{2}) =& v(t) + \frac{\Delta t}{2} \cdot a(t) \\
r(t+\Delta t) =& r(t) + \Delta t \cdot v(t+\frac{\Delta t}{2}) \\
a(t+\Delta t) =& \frac{1}{m} \cdot F\left[r(t+\Delta t), v(t) + \lambda \cdot \Delta t \cdot a(t)\right] \\
v(t+\Delta t) =& v(t+\frac{\Delta t}{2}) + \frac{\Delta t}{2} \cdot a(t+\Delta t)
\end{aligned}
$$

where the parameter λ depends on the specific choice of DPD parameters, and needs to be tuned on a case-by-case basis. Specification of a *lambda* value is optional. If specified, the setting must be from 0.0 to 1.0. If not specified, a default value of 0.5 is used, which effectively reproduces the standard velocity-Verlet (VV) scheme. For more details, see *Groot*.

Fix *mvv/dpd* updates the position and velocity of each atom. It can be used with the *pair_style mdpd* command or other pair styles such as *pair dpd*.

Fix *mvv/edpd* updates the per-atom temperature, in addition to position and velocity, and must be used with the *pair_style edpd* command.

Fix *mvv/tdpd* updates the per-atom chemical concentration, in addition to position and velocity, and must be used with the *pair_style tdpd* command.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.92.4 Restrictions

This fix is part of the USER-MESO package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.92.5 Related commands

pair_style mdpd, *pair_style edpd*, *pair_style tdpd*

16.92.6 Default

The default value for the optional *lambda* parameter is 0.5.

(Groot) Groot and Warren, J Chem Phys, 107: 4423-4435 (1997). DOI: 10.1063/1.474784

16.93 fix neb command

16.93.1 Syntax

```
fix ID group-ID neb Kspring keyword value
```

- ID, group-ID are documented in *fix* command
- neb = style name of this fix command
- Kspring = spring constant for parallel nudging force (force/distance units or force units, see parallel keyword)
- zero or more keyword/value pairs may be appended
- keyword = *parallel* or *perp* or *end*

```
parallel value = neigh or ideal
  neigh = parallel nudging force based on distance to neighbor replicas␣
↪(Kspring = force/distance units)
  ideal = parallel nudging force based on interpolated ideal position␣
↪(Kspring = force units)
perp value = Kspring2
  Kspring2 = spring constant for perpendicular nudging force (force/distance␣
↪units)
end values = estyle Kspring3
  estyle = first or last or last/efirst or last/efirst/middle
    first = apply force to first replica
    last = apply force to last replica
    last/efirst = apply force to last replica and set its target energy to␣
↪that of first replica
    last/efirst/middle = same as last/efirst plus prevent middle replicas␣
↪having lower energy than first replica
  Kspring3 = spring constant for target energy term (1/distance units)
```

16.93.2 Examples

```
fix 1 active neb 10.0
fix 2 all neb 1.0 perp 1.0 end last
fix 2 all neb 1.0 perp 1.0 end first 1.0 end last 1.0
fix 1 all neb 1.0 parallel ideal end last/efirst 1
```

16.93.3 Description

Add nudging forces to atoms in the group for a multi-replica simulation run via the *neb* command to perform a nudged elastic band (NEB) calculation for finding the transition state. Hi-level explanations of NEB are given with the *neb* command and on the *Howto replica* doc page. The fix neb command must be used with the "neb" command and defines how inter-replica nudging forces are computed. A NEB calculation is divided in two stages. In the first stage n replicas are relaxed toward a MEP until convergence. In the second stage, the climbing image scheme (see *(Henkelman2)*) is enabled, so that the replica having the highest energy relaxes toward the saddle point (i.e. the point of highest energy along the MEP), and a second relaxation is performed.

A key purpose of the nudging forces is to keep the replicas equally spaced. During the NEB calculation, the 3N-length vector of interatomic force Fi = -Grad(V) for each replica I is altered. For all intermediate replicas (i.e. for 1 < I < N, except the climbing replica) the force vector becomes:

```
Fi = -Grad(V) + (Grad(V) dot T') T' + Fnudge_parallel + Fnudge_perp
```

T' is the unit "tangent" vector for replica I and is a function of Ri, Ri-1, Ri+1, and the potential energy of the 3 replicas; it points roughly in the direction of (Ri+i - Ri-1); see the *(Henkelman1)* paper for details. Ri are the atomic coordinates of replica I; Ri-1 and Ri+1 are the coordinates of its neighbor replicas. The term (Grad(V) dot T') is used to remove the component of the gradient parallel to the path which would tend to distribute the replica unevenly along the path. Fnudge_parallel is an artificial nudging force which is applied only in the tangent direction and which maintains the equal spacing between replicas (see below for more information). Fnudge_perp is an optional artificial spring which is applied in a direction perpendicular to the tangent direction and which prevent the paths from forming acute kinks (see below for more information).

In the second stage of the NEB calculation, the interatomic force Fi for the climbing replica (the replica of highest energy after the first stage) is changed to:

```
Fi = -Grad(V) + 2 (Grad(V) dot T') T'
```

and the relaxation procedure is continued to a new converged MEP.

The keyword *parallel* specifies how the parallel nudging force is computed. With a value of *neigh*, the parallel nudging force is computed as in *(Henkelman1)* by connecting each intermediate replica with the previous and the next image:

```
Fnudge_parallel = Kspring * (|Ri+1 - Ri| - |Ri - Ri-1|)
```

Note that in this case the specified *Kspring* is in force/distance units.

With a value of *ideal*, the spring force is computed as suggested in ref`(WeinanE) <WeinanE>`

```
Fnudge_parallel = -Kspring * (RD-RDideal) / (2 * meanDist)
```

where RD is the "reaction coordinate" see *neb* section, and RDideal is the ideal RD for which all the images are equally spaced. I.e. RDideal = (I-1)*meanDist when the climbing replica is off, where I is the replica number). The meanDist is the average distance between replicas. Note that in this case the specified *Kspring* is in force units.

Note that the *ideal* form of nudging can often be more effective at keeping the replicas equally spaced.

The keyword *perp* specifies if and how a perpendicular nudging force is computed. It adds a spring force perpendicular to the path in order to prevent the path from becoming too strongly kinked. It can significantly improve the convergence of the NEB calculation when the resolution is poor. I.e. when few replicas are used; see *(Maras)* for details.

The perpendicular spring force is given by

```
Fnudge_perp = Kspring2 * F(Ri-1,Ri,Ri+1) (Ri+1 + Ri-1 - 2 Ri)
```

where *Kspring2* is the specified value. F(Ri-1 Ri R+1) is a smooth scalar function of the angle Ri-1 Ri Ri+1. It is equal to 0.0 when the path is straight and is equal to 1 when the angle Ri-1 Ri Ri+1 is acute. F(Ri-1 Ri R+1) is defined in *(Jonsson)*.

If *Kspring2* is set to 0.0 (the default) then no perpendicular spring force is added.

By default, no additional forces act on the first and last replicas during the NEB relaxation, so these replicas simply relax toward their respective local minima. By using the key word *end*, additional forces can be applied to the first and/or last replicas, to enable them to relax toward a MEP while constraining their energy E to the target energy ETarget.

If ETarget>E, the interatomic force Fi for the specified replica becomes:

```
Fi = -Grad(V) + (Grad(V) dot T' + (E-ETarget)*Kspring3) T',  when Grad(V) dot␣
↪T' < 0
Fi = -Grad(V) + (Grad(V) dot T' + (ETarget- E)*Kspring3) T', when Grad(V) dot␣
↪T' > 0
```

The "spring" constant on the difference in energies is the specified *Kspring3* value.

When *estyle* is specified as *first*, the force is applied to the first replica. When *estyle* is specified as *last*, the force is applied to the last replica. Note that the *end* keyword can be used twice to add forces to both the first and last replicas.

For both these *estyle* settings, the target energy *ETarget* is set to the initial energy of the replica (at the start of the NEB calculation).

If the *estyle* is specified as *last/efirst* or *last/efirst/middle*, force is applied to the last replica, but the target energy *ETarget* is continuously set to the energy of the first replica, as it evolves during the NEB relaxation.

The difference between these two *estyle* options is as follows. When *estyle* is specified as *last/efirst*, no change is made to the inter-replica force applied to the intermediate replicas (neither first or last). If the initial path is too far from the MEP, an intermediate replica may relax "faster" and reach a lower energy than the last replica. In this case the intermediate replica will be relaxing toward its own local minima. This behavior can be prevented by specifying *estyle* as *last/efirst/middle* which will alter the inter-replica force applied to intermediate replicas by removing the contribution of the gradient to the inter-replica force. This will only be done if a particular intermediate replica has a lower energy than the first replica. This should effectively prevent the intermediate replicas from over-relaxing.

After converging a NEB calculation using an *estyle* of *last/efirst/middle*, you should check that all intermediate replicas have a larger energy than the first replica. If this is not the case, the path is probably not a MEP.

Finally, note that the last replica may never reach the target energy if it is stuck in a local minima which has a larger energy than the target energy.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, as invoked by the *minimize* command via the *neb* command.

16.93.4 Restrictions

This command can only be used if LAMMPS was built with the REPLICA package. See the *Build package* doc page for more info.

16.93.5 Related commands

neb

16.93.6 Default

The option defaults are parallel = neigh, perp = 0.0, ends is not specified (no inter-replica force on the end replicas).

(Henkelman1) Henkelman and Jonsson, J Chem Phys, 113, 9978-9985 (2000).

(Henkelman2) Henkelman, Uberuaga, Jonsson, J Chem Phys, 113, 9901-9904 (2000).

(WeinanE) E, Ren, Vanden-Eijnden, Phys Rev B, 66, 052301 (2002).

(Jonsson) Jonsson, Mills and Jacobsen, in Classical and Quantum Dynamics in Condensed Phase Simulations, edited by Berne, Ciccotti, and Coker World Scientific, Singapore, 1998, p 385.

(Maras) Maras, Trushin, Stukowski, Ala-Nissila, Jonsson, Comp Phys Comm, 205, 13-21 (2016).

16.94 fix neb/spin command

16.94.1 Syntax

```
fix ID group-ID neb/spin Kspring
```

- ID, group-ID are documented in *fix* command
- neb/spin = style name of this fix command

```
Kspring = spring constant for parallel nudging force
(force/distance units or force units, see parallel keyword)
```

16.94.2 Examples

fix 1 active neb/spin 1.0

16.94.3 Description

Add nudging forces to spins in the group for a multi-replica simulation run via the *neb/spin* command to perform a geodesic nudged elastic band (GNEB) calculation for finding the transition state. Hi-level explanations of GNEB are given with the *neb/spin* command and on the *Howto replica* doc page. The fix neb/spin command must be used with the "neb/spin" command and defines how inter-replica nudging forces are computed. A GNEB calculation is divided in two stages. In the first stage n replicas are relaxed toward a MEP until convergence. In the second stage, the climbing image scheme is enabled, so that the replica having the highest energy relaxes toward the saddle point (i.e. the point of highest energy along the MEP), and a second relaxation is performed.

The nudging forces are calculated as explained in *(BessarabB)*). See this reference for more explanation about their expression.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, as invoked by the *minimize* command via the *neb/spin* command.

16.94.4 Restrictions

This command can only be used if LAMMPS was built with the SPIN package. See the *Build package* doc page for more info.

16.94.5 Related commands

neb_spin

16.94.6 Default

none

(BessarabB) Bessarab, Uzdin, Jonsson, Comp Phys Comm, 196, 335-347 (2015).

16.95 fix nvt command

16.96 fix nvt/intel command

16.97 fix nvt/kk command

16.98 fix nvt/omp command

16.99 fix npt command

16.100 fix npt/intel command

16.101 fix npt/kk command

16.102 fix npt/omp command

16.103 fix nph command

16.104 fix nph/kk command

16.105 fix nph/omp command

16.105.1 Syntax

```
fix ID group-ID style_name keyword value ...
```

- ID, group-ID are documented in *fix* command
- style_name = *nvt* or *npt* or *nph*
- one or more keyword/value pairs may be appended

```
keyword = temp or iso or aniso or tri or x or y or z or xy or yz or xz␣
↪or couple or tchain or pchain or mtk or tloop or ploop or nreset or␣
↪drag or dilate or scalexy or scaleyz or scalexz or flip or fixedpoint␣
↪or update
  temp values = Tstart Tstop Tdamp
    Tstart,Tstop = external temperature at start/end of run
    Tdamp = temperature damping parameter (time units)
  iso or aniso or tri values = Pstart Pstop Pdamp
    Pstart,Pstop = scalar external pressure at start/end of run (pressure␣
↪units)
    Pdamp = pressure damping parameter (time units)
  x or y or z or xy or yz or xz values = Pstart Pstop Pdamp
    Pstart,Pstop = external stress tensor component at start/end of run␣
↪(pressure units)
```

```
    Pdamp = stress damping parameter (time units)
  couple = none or xyz or xy or yz or xz
  tchain value = N
    N = length of thermostat chain (1 = single thermostat)
  pchain values = N
    N length of thermostat chain on barostat (0 = no thermostat)
  mtk value = yes or no = add in MTK adjustment term or not
  tloop value = M
    M = number of sub-cycles to perform on thermostat
  ploop value = M
    M = number of sub-cycles to perform on barostat thermostat
  nreset value = reset reference cell every this many timesteps
  drag value = Df
    Df = drag factor added to barostat/thermostat (0.0 = no drag)
  dilate value = dilate-group-ID
    dilate-group-ID = only dilate atoms in this group due to barostat␣
↪volume changes
  scalexy value = yes or no = scale xy with ly
  scaleyz value = yes or no = scale yz with lz
  scalexz value = yes or no = scale xz with lz
  flip value = yes or no = allow or disallow box flips when it becomes␣
↪highly skewed
  fixedpoint values = x y z
    x,y,z = perform barostat dilation/contraction around this point␣
↪(distance units)
  update value = dipole or dipole/dlm
    dipole = update dipole orientation (only for sphere variants)
    dipole/dlm = use DLM integrator to update dipole orientation (only␣
↪for sphere variants)
```

16.105.2 Examples

```
fix 1 all nvt temp 300.0 300.0 100.0
fix 1 water npt temp 300.0 300.0 100.0 iso 0.0 0.0 1000.0
fix 2 jello npt temp 300.0 300.0 100.0 tri 5.0 5.0 1000.0
fix 2 ice nph x 1.0 1.0 0.5 y 2.0 2.0 0.5 z 3.0 3.0 0.5 yz 0.1 0.1 0.5 xz 0.2 0.2 0.5␣
↪xy 0.3 0.3 0.5 nreset 1000
```

16.105.3 Description

These commands perform time integration on Nose-Hoover style non-Hamiltonian equations of motion which are designed to generate positions and velocities sampled from the canonical (nvt), isothermal-isobaric (npt), and isenthalpic (nph) ensembles. This updates the position and velocity for atoms in the group each timestep.

The thermostatting and barostatting is achieved by adding some dynamic variables which are coupled to the particle velocities (thermostatting) and simulation domain dimensions (barostatting). In addition to basic thermostatting and barostatting, these fixes can also create a chain of thermostats coupled to the particle thermostat, and another chain of thermostats coupled to the barostat variables. The barostat can be coupled to the overall box volume, or to individual dimensions, including the *xy*, *xz* and *yz* tilt dimensions. The external pressure of the barostat can be specified as either a scalar pressure (isobaric ensemble) or as components of a symmetric stress tensor (constant stress ensemble). When used correctly, the time-averaged temperature and stress tensor of the particles will match the target values specified by Tstart/Tstop and Pstart/Pstop.

The equations of motion used are those of Shinoda et al in *(Shinoda)*, which combine the hydrostatic equations of Martyna, Tobias and Klein in *(Martyna)* with the strain energy proposed by Parrinello and Rahman in *(Parrinello)*. The time integration schemes closely follow the time-reversible measure-preserving Verlet and rRESPA integrators derived by Tuckerman et al in *(Tuckerman)*.

The thermostat parameters for fix styles *nvt* and *npt* are specified using the *temp* keyword. Other thermostat-related keywords are *tchain*, *tloop* and *drag*, which are discussed below.

The thermostat is applied to only the translational degrees of freedom for the particles. The translational degrees of freedom can also have a bias velocity removed before thermostatting takes place; see the description below. The desired temperature at each timestep is a ramped value during the run from *Tstart* to *Tstop*. The *Tdamp* parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 10.0 means to relax the temperature in a timespan of (roughly) 10 time units (e.g. tau or fmsec or psec - see the *units* command). The atoms in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the integration.

Note: A Nose-Hoover thermostat will not work well for arbitrary values of *Tdamp*. If *Tdamp* is too small, the temperature can fluctuate wildly; if it is too large, the temperature will take a very long time to equilibrate. A good choice for many models is a *Tdamp* of around 100 timesteps. Note that this is NOT the same as 100 time units for most *units* settings. A simple way to ensure this, is via using an *immediate variable* expression accessing the thermo property 'dt', which is the length of the time step. Example:

```
fix 1 all nvt temp 300.0 300.0 $(100.0*dt)
```

The barostat parameters for fix styles *npt* and *nph* is specified using one or more of the *iso*, *aniso*, *tri*, *x*, *y*, *z*, *xy*, *xz*, *yz*, and *couple* keywords. These keywords give you the ability to specify all 6 components of an external stress tensor, and to couple various of these components together so that the dimensions they represent are varied together during a constant-pressure simulation.

Other barostat-related keywords are *pchain*, *mtk*, *ploop*, *nreset*, *drag*, and *dilate*, which are discussed below.

Orthogonal simulation boxes have 3 adjustable dimensions (x,y,z). Triclinic (non-orthogonal) simulation boxes have 6 adjustable dimensions (x,y,z,xy,xz,yz). The *create_box*, *read data*, and *read_restart* commands specify whether the simulation box is orthogonal or non-orthogonal (triclinic) and explain the meaning of the xy,xz,yz tilt factors.

The target pressures for each of the 6 components of the stress tensor can be specified independently via the *x*, *y*, *z*, *xy*, *xz*, *yz* keywords, which correspond to the 6 simulation box dimensions. For each component, the external pressure or tensor component at each timestep is a ramped value during the run from *Pstart* to *Pstop*. If a target pressure is specified for a component, then the corresponding box dimension will change during a simulation. For example, if the *y* keyword is used, the y-box length will change. If the *xy* keyword is used, the xy tilt factor will change. A box dimension will not change if that component is not specified, although you have the option to change that dimension via the *fix deform* command.

Note that in order to use the *xy*, *xz*, or *yz* keywords, the simulation box must be triclinic, even if its initial tilt factors are 0.0.

For all barostat keywords, the *Pdamp* parameter operates like the *Tdamp* parameter, determining the time scale on which pressure is relaxed. For example, a value of 10.0 means to relax the pressure in a timespan of (roughly) 10 time units (e.g. tau or fmsec or psec - see the *units* command).

Note: A Nose-Hoover barostat will not work well for arbitrary values of *Pdamp*. If *Pdamp* is too small, the pressure and volume can fluctuate wildly; if it is too large, the pressure will take a very long time to equilibrate. A good choice

for many models is a *Pdamp* of around 1000 timesteps. However, note that *Pdamp* is specified in time units, and that timesteps are NOT the same as time units for most *units* settings.

Regardless of what atoms are in the fix group (the only atoms which are time integrated), a global pressure or stress tensor is computed for all atoms. Similarly, when the size of the simulation box is changed, all atoms are re-scaled to new positions, unless the keyword *dilate* is specified with a *dilate-group-ID* for a group that represents a subset of the atoms. This can be useful, for example, to leave the coordinates of atoms in a solid substrate unchanged and controlling the pressure of a surrounding fluid. This option should be used with care, since it can be unphysical to dilate some atoms and not others, because it can introduce large, instantaneous displacements between a pair of atoms (one dilated, one not) that are far from the dilation origin. Also note that for atoms not in the fix group, a separate time integration fix like *fix nve* or *fix nvt* can be used on them, independent of whether they are dilated or not.

The *couple* keyword allows two or three of the diagonal components of the pressure tensor to be "coupled" together. The value specified with the keyword determines which are coupled. For example, *xz* means the *Pxx* and *Pzz* components of the stress tensor are coupled. *Xyz* means all 3 diagonal components are coupled. Coupling means two things: the instantaneous stress will be computed as an average of the corresponding diagonal components, and the coupled box dimensions will be changed together in lockstep, meaning coupled dimensions will be dilated or contracted by the same percentage every timestep. The *Pstart*, *Pstop*, *Pdamp* parameters for any coupled dimensions must be identical. *Couple xyz* can be used for a 2d simulation; the *z* dimension is simply ignored.

The *iso*, *aniso*, and *tri* keywords are simply shortcuts that are equivalent to specifying several other keywords together.

The keyword *iso* means couple all 3 diagonal components together when pressure is computed (hydrostatic pressure), and dilate/contract the dimensions together. Using "iso Pstart Pstop Pdamp" is the same as specifying these 4 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
couple xyz
```

The keyword *aniso* means *x*, *y*, and *z* dimensions are controlled independently using the *Pxx*, *Pyy*, and *Pzz* components of the stress tensor as the driving forces, and the specified scalar external pressure. Using "aniso Pstart Pstop Pdamp" is the same as specifying these 4 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
couple none
```

The keyword *tri* means *x*, *y*, *z*, *xy*, *xz*, and *yz* dimensions are controlled independently using their individual stress components as the driving forces, and the specified scalar pressure as the external normal stress. Using "tri Pstart Pstop Pdamp" is the same as specifying these 7 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
xy 0.0 0.0 Pdamp
yz 0.0 0.0 Pdamp
xz 0.0 0.0 Pdamp
couple none
```

In some cases (e.g. for solids) the pressure (volume) and/or temperature of the system can oscillate undesirably when a Nose/Hoover barostat and thermostat is applied. The optional *drag* keyword will damp these oscillations, although it alters the Nose/Hoover equations. A value of 0.0 (no drag) leaves the Nose/Hoover formalism unchanged. A non-zero value adds a drag term; the larger the value specified, the greater the damping effect. Performing a short run and monitoring the pressure and temperature is the best way to determine if the drag term is working. Typically a value between 0.2 to 2.0 is sufficient to damp oscillations after a few periods. Note that use of the drag keyword will interfere with energy conservation and will also change the distribution of positions and velocities so that they do not correspond to the nominal NVT, NPT, or NPH ensembles.

An alternative way to control initial oscillations is to use chain thermostats. The keyword *tchain* determines the number of thermostats in the particle thermostat. A value of 1 corresponds to the original Nose-Hoover thermostat. The keyword *pchain* specifies the number of thermostats in the chain thermostatting the barostat degrees of freedom. A value of 0 corresponds to no thermostatting of the barostat variables.

The *mtk* keyword controls whether or not the correction terms due to Martyna, Tuckerman, and Klein are included in the equations of motion *(Martyna)*. Specifying *no* reproduces the original Hoover barostat, whose volume probability distribution function differs from the true NPT and NPH ensembles by a factor of 1/V. Hence using *yes* is more correct, but in many cases the difference is negligible.

The keyword *tloop* can be used to improve the accuracy of integration scheme at little extra cost. The initial and final updates of the thermostat variables are broken up into *tloop* sub-steps, each of length *dt*/*tloop*. This corresponds to using a first-order Suzuki-Yoshida scheme *(Tuckerman)*. The keyword *ploop* does the same thing for the barostat thermostat.

The keyword *nreset* controls how often the reference dimensions used to define the strain energy are reset. If this keyword is not used, or is given a value of zero, then the reference dimensions are set to those of the initial simulation domain and are never changed. If the simulation domain changes significantly during the simulation, then the final average pressure tensor will differ significantly from the specified values of the external stress tensor. A value of *nstep* means that every *nstep* timesteps, the reference dimensions are set to those of the current simulation domain.

The *scaleyz*, *scalexz*, and *scalexy* keywords control whether or not the corresponding tilt factors are scaled with the associated box dimensions when barostatting triclinic periodic cells. The default values *yes* will turn on scaling, which corresponds to adjusting the linear dimensions of the cell while preserving its shape. Choosing *no* ensures that the tilt factors are not scaled with the box dimensions. See below for restrictions and default values in different situations. In older versions of LAMMPS, scaling of tilt factors was not performed. The old behavior can be recovered by setting all three scale keywords to *no*.

The *flip* keyword allows the tilt factors for a triclinic box to exceed half the distance of the parallel box length, as discussed below. If the *flip* value is set to *yes*, the bound is enforced by flipping the box when it is exceeded. If the *flip* value is set to *no*, the tilt will continue to change without flipping. Note that if applied stress induces large deformations (e.g. in a liquid), this means the box shape can tilt dramatically and LAMMPS will run less efficiently, due to the large volume of communication needed to acquire ghost atoms around a processor's irregular-shaped sub-domain. For extreme values of tilt, LAMMPS may also lose atoms and generate an error.

The *fixedpoint* keyword specifies the fixed point for barostat volume changes. By default, it is the center of the box. Whatever point is chosen will not move during the simulation. For example, if the lower periodic boundaries pass through (0,0,0), and this point is provided to *fixedpoint*, then the lower periodic boundaries will remain at (0,0,0), while the upper periodic boundaries will move twice as far. In all cases, the particle trajectories are unaffected by the chosen value, except for a time-dependent constant translation of positions.

If the *update* keyword is used with the *dipole* value, then the orientation of the dipole moment of each particle is also updated during the time integration. This option should be used for models where a dipole moment is assigned to finite-size particles, e.g. spheroids via use of the *atom_style hybrid sphere dipole* command.

The default dipole orientation integrator can be changed to the Dullweber-Leimkuhler-McLachlan integration scheme *(Dullweber)* when using *update* with the value *dipole/dlm*. This integrator is symplectic and time-reversible, giving better energy conservation and allows slightly longer timesteps at only a small additional computational cost.

Note: Using a barostat coupled to tilt dimensions *xy*, *xz*, *yz* can sometimes result in arbitrarily large values of the tilt dimensions, i.e. a dramatically deformed simulation box. LAMMPS allows the tilt factors to grow a small amount beyond the normal limit of half the box length (0.6 times the box length), and then performs a box "flip" to an equivalent periodic cell. See the discussion of the *flip* keyword above, to allow this bound to be exceeded, if desired.

The flip operation is described in more detail in the doc page for *fix deform*. Both the barostat dynamics and the atom trajectories are unaffected by this operation. However, if a tilt factor is incremented by a large amount (1.5 times the box length) on a single timestep, LAMMPS can not accommodate this event and will terminate the simulation with an error. This error typically indicates that there is something badly wrong with how the simulation was constructed, such as specifying values of *Pstart* that are too far from the current stress value, or specifying a timestep that is too large. Triclinic barostatting should be used with care. This also is true for other barostat styles, although they tend to be more forgiving of insults. In particular, it is important to recognize that equilibrium liquids can not support a shear stress and that equilibrium solids can not support shear stresses that exceed the yield stress.

One exception to this rule is if the 1st dimension in the tilt factor (x for xy) is non-periodic. In that case, the limits on the tilt factor are not enforced, since flipping the box in that dimension does not change the atom positions due to non-periodicity. In this mode, if you tilt the system to extreme angles, the simulation will simply become inefficient due to the highly skewed simulation box.

Note: Unlike the *fix temp/berendsen* command which performs thermostatting but NO time integration, these fixes perform thermostatting/barostatting AND time integration. Thus you should not use any other time integration fix, such as *fix nve* on atoms to which this fix is applied. Likewise, fix nvt and fix npt should not normally be used on atoms that also have their temperature controlled by another fix - e.g. by *fix langevin* or *fix temp/rescale* commands.

See the *Howto thermostat* and *Howto barostat* doc pages for a discussion of different ways to compute temperature and perform thermostatting and barostatting.

These fixes compute a temperature and pressure each timestep. To do this, the thermostat and barostat fixes create their own computes of style "temp" and "pressure", as if one of these sets of commands had been issued:

For fix nvt: compute fix-ID_temp group-ID temp

```
For fix npt and fix nph:
compute fix-ID_temp all temp
compute fix-ID_press all pressure fix-ID_temp
```

For fix nvt, the group for the new temperature compute is the same as the fix group. For fix npt and fix nph, the group for both the new temperature and pressure compute is "all" since pressure is computed for the entire system. In the case of fix nph, the temperature compute is not used for thermostatting, but just for a kinetic-energy contribution to the pressure. See the *compute temp* and *compute pressure* commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press".

Note that these are NOT the computes used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of these fix's temperature or pressure via the *compute_modify* command. Or you can print this temperature or pressure during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Like other fixes that perform thermostatting, fix nvt and fix npt can be used with *compute commands* that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in

a geometric region. This is not done by default, but only if the *fix_modify* command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual *compute commands* to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

These fixes can be used with either the *verlet* or *respa integrators*. When using one of the barostat fixes with *respa*, LAMMPS uses an integrator constructed according to the following factorization of the Liouville propagator (for two rRESPA levels):

$$\begin{aligned}\exp\left(\mathrm{i}L\Delta t\right) =& \hat{E}\exp\left(\mathrm{i}L_{\text{T-baro}}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_{\text{T-part}}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_{\epsilon,2}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_2^{(2)}\frac{\Delta t}{2}\right)\\ &\times\left[\exp\left(\mathrm{i}L_2^{(1)}\frac{\Delta t}{2n}\right)\exp\left(\mathrm{i}L_{\epsilon,1}\frac{\Delta t}{2n}\right)\exp\left(\mathrm{i}L_1\frac{\Delta t}{n}\right)\exp\left(\mathrm{i}L_{\epsilon,1}\frac{\Delta t}{2n}\right)\exp\left(\mathrm{i}L_2^{(1)}\frac{\Delta t}{2n}\right)\right]^n\\ &\times\exp\left(\mathrm{i}L_2^{(2)}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_{\epsilon,2}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_{\text{T-part}}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_{\text{T-baro}}\frac{\Delta t}{2}\right)\\ &+\mathcal{O}\left(\Delta t^3\right)\end{aligned}$$

This factorization differs somewhat from that of Tuckerman et al, in that the barostat is only updated at the outermost rRESPA level, whereas Tuckerman's factorization requires splitting the pressure into pieces corresponding to the forces computed at each rRESPA level. In theory, the latter method will exhibit better numerical stability. In practice, because Pdamp is normally chosen to be a large multiple of the outermost rRESPA timestep, the barostat dynamics are not the limiting factor for numerical stability. Both factorizations are time-reversible and can be shown to preserve the phase space measure of the underlying non-Hamiltonian equations of motion.

Note: This implementation has been shown to conserve linear momentum up to machine precision under NVT dynamics. Under NPT dynamics, for a system with zero initial total linear momentum, the total momentum fluctuates close to zero. It may occasionally undergo brief excursions to non-negligible values, before returning close to zero. Over long simulations, this has the effect of causing the center-of-mass to undergo a slow random walk. This can be mitigated by resetting the momentum at infrequent intervals using the *fix momentum* command.

The fix npt and fix nph commands can be used with rigid bodies or mixtures of rigid bodies and non-rigid particles (e.g. solvent). But there are also *fix rigid/npt* and *fix rigid/nph* commands, which are typically a more natural choice. See the doc page for those commands for more discussion of the various ways to do this.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

These fixes writes the state of all the thermostat and barostat variables to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify* *temp* and *press* options are supported by these fixes. You can use them to assign a *compute* you have defined to this fix which will be used in its thermostatting or barostatting procedure, as described above. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

Note: If both the *temp* and *press* keywords are used in a single thermo_modify command (or in two separate commands), then the order in which the keywords are specified is important. Note that a *pressure compute* defines its own temperature compute as an argument when it is specified. The *temp* keyword will override this (for the pressure compute being used by fix npt), but only if the *temp* keyword comes after the *press* keyword. If the *temp* keyword comes before the *press* keyword, then the new pressure compute specified by the *press* keyword will be unaffected by the *temp* setting.

The *fix_modify* *energy* option is supported by these fixes to add the energy change induced by Nose/Hoover thermostatting and barostatting to the system's potential energy as part of *thermodynamic output*.

These fixes compute a global scalar and a global vector of quantities, which can be accessed by various *output commands*. The scalar value calculated by these fixes is "extensive"; the vector values are "intensive".

The scalar is the cumulative energy change due to the fix.

The vector stores internal Nose/Hoover thermostat and barostat variables. The number and meaning of the vector values depends on which fix is used and the settings for keywords *tchain* and *pchain*, which specify the number of Nose/Hoover chains for the thermostat and barostat. If no thermostatting is done, then *tchain* is 0. If no barostatting is done, then *pchain* is 0. In the following list, "ndof" is 0, 1, 3, or 6, and is the number of degrees of freedom in the barostat. Its value is 0 if no barostat is used, else its value is 6 if any off-diagonal stress tensor component is barostatted, else its value is 1 if *couple xyz* is used or *couple xy* for a 2d simulation, otherwise its value is 3.

The order of values in the global vector and their meaning is as follows. The notation means there are tchain values for eta, followed by tchain for eta_dot, followed by ndof for omega, etc:

- eta[tchain] = particle thermostat displacements (unitless)
- eta_dot[tchain] = particle thermostat velocities (1/time units)
- omega[ndof] = barostat displacements (unitless)
- omega_dot[ndof] = barostat velocities (1/time units)
- etap[pchain] = barostat thermostat displacements (unitless)
- etap_dot[pchain] = barostat thermostat velocities (1/time units)
- PE_eta[tchain] = potential energy of each particle thermostat displacement (energy units)
- KE_eta_dot[tchain] = kinetic energy of each particle thermostat velocity (energy units)
- PE_omega[ndof] = potential energy of each barostat displacement (energy units)
- KE_omega_dot[ndof] = kinetic energy of each barostat velocity (energy units)
- PE_etap[pchain] = potential energy of each barostat thermostat displacement (energy units)
- KE_etap_dot[pchain] = kinetic energy of each barostat thermostat velocity (energy units)
- PE_strain[1] = scalar strain energy (energy units)

These fixes can ramp their external temperature and pressure over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

These fixes are not invoked during *energy minimization*.

16.105.4 Restrictions

X, *y*, *z* cannot be barostatted if the associated dimension is not periodic. *Xy*, *xz*, and *yz* can only be barostatted if the simulation domain is triclinic and the 2nd dimension in the keyword (*y* dimension in *xy*) is periodic. *Z*, *xz*, and *yz*, cannot be barostatted for 2D simulations. The *create_box*, *read data*, and *read_restart* commands specify whether the simulation box is orthogonal or non-orthogonal (triclinic) and explain the meaning of the xy,xz,yz tilt factors.

For the *temp* keyword, the final Tstop cannot be 0.0 since it would make the external T = 0.0 at some timestep during the simulation which is not allowed in the Nose/Hoover formulation.

The *scaleyz yes* and *scalexz yes* keyword/value pairs can not be used for 2D simulations. *scaleyz yes*, *scalexz yes*, and *scalexy yes* options can only be used if the 2nd dimension in the keyword is periodic, and if the tilt factor is not coupled to the barostat via keywords *tri*, *yz*, *xz*, and *xy*.

These fixes can be used with dynamic groups as defined by the *group* command. Likewise they can be used with groups to which atoms are added or deleted over time, e.g. a deposition simulation. However, the conservation properties of the thermostat and barostat are defined for systems with a static set of atoms. You may observe odd behavior if the atoms in a group vary dramatically over time or the atom count becomes very small.

16.105.5 Related commands

fix nve, *fix_modify*, *run_style*

16.105.6 Default

The keyword defaults are tchain = 3, pchain = 3, mtk = yes, tloop = 1, ploop = 1, nreset = 0, drag = 0.0, dilate = all, couple = none, flip = yes, scaleyz = scalexz = scalexy = yes if periodic in 2nd dimension and not coupled to barostat, otherwise no.

(Martyna) Martyna, Tobias and Klein, J Chem Phys, 101, 4177 (1994).

(Parrinello) Parrinello and Rahman, J Appl Phys, 52, 7182 (1981).

(Tuckerman) Tuckerman, Alejandre, Lopez-Rendon, Jochim, and Martyna, J Phys A: Math Gen, 39, 5629 (2006).

(Shinoda) Shinoda, Shiga, and Mikami, Phys Rev B, 69, 134103 (2004).

(Dullweber) Dullweber, Leimkuhler and McLachlan, J Chem Phys, 107, 5840 (1997).

16.106 fix nvt/eff command

16.107 fix npt/eff command

16.108 fix nph/eff command

16.108.1 Syntax

```
fix ID group-ID style_name keyword value ...
```

- ID, group-ID are documented in *fix* command
- style_name = *nvt/eff* or *npt/eff* or *nph/eff*

```
one or more keyword value pairs may be appended
keyword = temp or iso or aniso or tri or x or y or z or xy or yz or xz␣
↪or couple or tchain or pchain or mtk or tloop or ploop or nreset or␣
↪drag or dilate
  temp values = Tstart Tstop Tdamp
    Tstart,Tstop = external temperature at start/end of run
    Tdamp = temperature damping parameter (time units)
  iso or aniso or tri values = Pstart Pstop Pdamp
    Pstart,Pstop = scalar external pressure at start/end of run (pressure␣
↪units)
    Pdamp = pressure damping parameter (time units)
  x or y or z or xy or yz or xz values = Pstart Pstop Pdamp
    Pstart,Pstop = external stress tensor component at start/end of run␣
↪(pressure units)
    Pdamp = stress damping parameter (time units)
  couple = none or xyz or xy or yz or xz
  tchain value = length of thermostat chain (1 = single thermostat)
  pchain values = length of thermostat chain on barostat (0 = no␣
↪thermostat)
  mtk value = yes or no = add in MTK adjustment term or not
  tloop value = number of sub-cycles to perform on thermostat
  ploop value = number of sub-cycles to perform on barostat thermostat
  nreset value = reset reference cell every this many timesteps
  drag value = drag factor added to barostat/thermostat (0.0 = no drag)
  dilate value = all or partial
```

16.108.2 Examples

```
fix 1 all nvt/eff temp 300.0 300.0 0.1
fix 1 part npt/eff temp 300.0 300.0 0.1 iso 0.0 0.0 1.0
fix 2 part npt/eff temp 300.0 300.0 0.1 tri 5.0 5.0 1.0
fix 2 ice nph/eff x 1.0 1.0 0.5 y 2.0 2.0 0.5 z 3.0 3.0 0.5 yz 0.1 0.1 0.5 xz 0.2 0.2␣
↪0.5 xy 0.3 0.3 0.5 nreset 1000
```

16.108.3 Description

These commands perform time integration on Nose-Hoover style non-Hamiltonian equations of motion for nuclei and electrons in the group for the *electron force field* model. The fixes are designed to generate positions and velocities sampled from the canonical (nvt), isothermal-isobaric (npt), and isenthalpic (nph) ensembles. This is achieved by adding some dynamic variables which are coupled to the particle velocities (thermostatting) and simulation domain dimensions (barostatting). In addition to basic thermostatting and barostatting, these fixes can also create a chain of thermostats coupled to the particle thermostat, and another chain of thermostats coupled to the barostat variables. The barostat can be coupled to the overall box volume, or to individual dimensions, including the *xy*, *xz* and *yz* tilt dimensions. The external pressure of the barostat can be specified as either a scalar pressure (isobaric ensemble) or as components of a symmetric stress tensor (constant stress ensemble). When used correctly, the time-averaged temperature and stress tensor of the particles will match the target values specified by Tstart/Tstop and Pstart/Pstop.

The operation of these fixes is exactly like that described by the *fix nvt, npt, and nph* commands, except that the radius and radial velocity of electrons are also updated. Likewise the temperature and pressure calculated by the fix, using the computes it creates (as discussed in the *fix nvt, npt, and nph* doc page), are performed with computes that include the eFF contribution to the temperature or kinetic energy from the electron radial velocity.

Note: there are two different pressures that can be reported for eFF when defining the pair_style (see *pair eff/cut* to understand these settings), one (default) that considers electrons do not contribute radial virial components (i.e. electrons treated as incompressible 'rigid' spheres) and one that does. The radial electronic contributions to the virials are only tallied if the flexible pressure option is set, and this will affect both global and per-atom quantities. In principle, the true pressure of a system is somewhere in between the rigid and the flexible eFF pressures, but, for most cases, the difference between these two pressures will not be significant over long-term averaged runs (i.e. even though the energy partitioning changes, the total energy remains similar).

Note: currently, there is no available option for the user to set or create temperature distributions that include the radial electronic degrees of freedom with the *velocity* command, so the the user must allow for these degrees of freedom to equilibrate (i.e. equi-partitioning of energy) through time integration.

Restart, fix_modify, output, run start/stop, minimize info:

See the doc page for the *fix nvt, npt, and nph* commands for details.

16.108.4 Restrictions

This fix is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Other restriction discussed on the doc page for the *fix nvt, npt, and nph* commands also apply.

Note: The temperature for systems (regions or groups) with only electrons and no nuclei is 0.0 (i.e. not defined) in the current temperature calculations, a practical example would be a uniform electron gas or a very hot plasma, where electrons remain delocalized from the nuclei. This is because, even though electron virials are included in the temperature calculation, these are averaged over the nuclear degrees of freedom only. In such cases a corrective term must be added to the pressure to get the correct kinetic contribution.

16.108.5 Related commands

fix nvt, *fix nph*, *fix npt*, *fix_modify*, *run_style*

16.108.6 Default

The keyword defaults are tchain = 3, pchain = 3, mtk = yes, tloop = ploop = 1, nreset = 0, drag = 0.0, dilate = all, and couple = none.

(Martyna) Martyna, Tobias and Klein, J Chem Phys, 101, 4177 (1994).

(Parrinello) Parrinello and Rahman, J Appl Phys, 52, 7182 (1981).

(Tuckerman) Tuckerman, Alejandre, Lopez-Rendon, Jochim, and Martyna, J Phys A: Math Gen, 39, 5629 (2006).

(Shinoda) Shinoda, Shiga, and Mikami, Phys Rev B, 69, 134103 (2004).

16.109 fix nvt/uef command

16.110 fix npt/uef command

16.110.1 Syntax

```
fix ID group-ID style_name erate edot_x edot_y temp Tstart Tstop Tdamp keyword value .
↪..
```

- ID, group-ID are documented in *fix* command
- style_name = *nvt/uef* or *npt/uef*
- *Tstart*, *Tstop*, and *Tdamp* are documented in the *fix npt* command
- *edot_x* and *edot_y* are the strain rates in the x and y directions (1/(time units))
- one or more keyword/value pairs may be appended

```
keyword = ext or strain or iso or x or y or z or tchain or pchain or␣
↪tloop or ploop or mtk
  ext value = x or y or z or xy or yz or xz = external dimensions
    sets the external dimensions used to calculate the scalar pressure
  strain values = e_x e_y = initial strain
    usually not needed, but may be needed to resume a run with a data␣
↪file.
  iso, x, y, z, tchain, pchain, tloop, ploop, mtk keywords
    documented by the fix npt command
```

16.110.2 Examples

```
fix uniax_nvt all nvt/uef temp 400 400 100 erate 0.00001 -0.000005
fix biax_nvt all nvt/uef temp 400 400 100 erate 0.000005 0.000005
fix uniax_npt all npt/uef temp 400 400 300 iso 1 1 3000 erate 0.00001 -0.000005 ext yz
fix biax_npt all npt/uef temp 400 400 100 erate -0.00001 0.000005 x 1 1 3000
```

16.110.3 Description

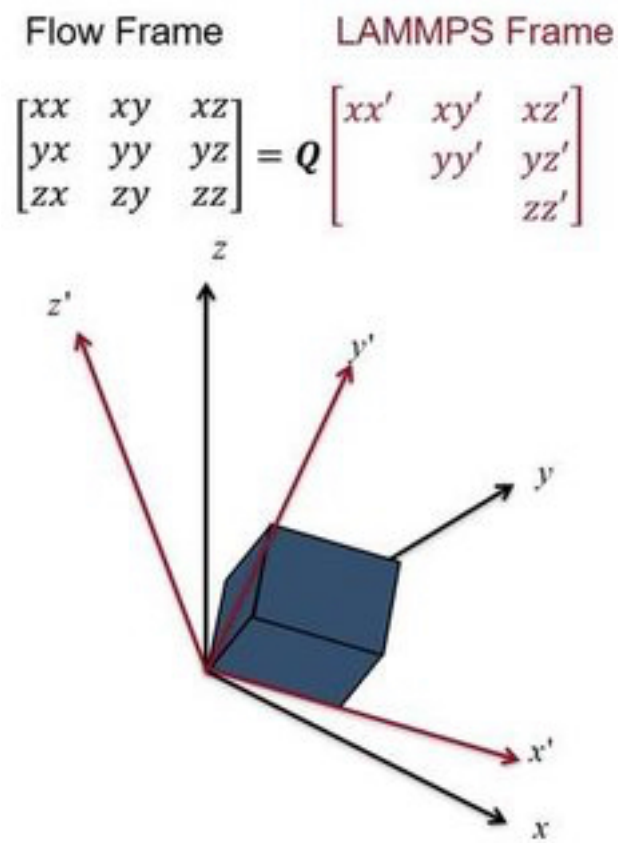
This fix can be used to simulate non-equilibrium molecular dynamics (NEMD) under diagonal flow fields, including uniaxial and bi-axial flow. Simulations under continuous extensional flow may be carried out for an indefinite amount of time. It is an implementation of the boundary conditions from *(Dobson)*, and also uses numerical lattice reduction as was proposed by *(Hunt)*. The lattice reduction algorithm is from *(Semaev)*. The fix is intended for simulations of homogeneous flows, and integrates the SLLOD equations of motion, originally proposed by Hoover and Ladd (see *(Evans and Morriss)*). Additional detail about this implementation can be found in *(Nicholson and Rutledge)*.

Note that NEMD simulations of a continuously strained system can be performed using the *fix deform*, *fix nvt/sllod*, and *compute temp/deform* commands.

The applied flow field is set by the *eps* keyword. The values *edot_x* and *edot_y* correspond to the strain rates in the xx and yy directions. It is implicitly assumed that the flow field is traceless, and therefore the strain rate in the zz direction is eqal to -(*edot_x* + *edot_y*).

Note: Due to an instability in the SLLOD equations under extension, *fix momentum* should be used to regularly reset the linear momentum.

The boundary conditions require a simulation box that does not have a consistent alignment relative to the applied flow field. Since LAMMPS utilizes an upper-triangular simulation box, it is not possible to express the evolving simulation box in the same coordinate system as the flow field. This fix keeps track of two coordinate systems: the flow frame, and the upper triangular LAMMPS frame. The coordinate systems are related to each other through the QR decomposition, as is illustrated in the image below.



During most molecular dynamics operations, the system is represented in the LAMMPS frame. Only when the positions and velocities are updated is the system rotated to the flow frame, and it is rotated back to the LAMMPS frame immediately afterwards. For this reason, all vector-valued quantities (except for the tensors from *compute pressure/uef* and *compute temp/uef*) will be computed in the LAMMPS frame. Rotationally invariant scalar quantities like the temperature and hydrostatic pressure are frame-invariant and will be computed correctly. Additionally, the system is in the LAMMPS frame during all of the output steps, and therefore trajectory files made using the dump command will be in the LAMMPS frame unless the *dump cfg/uef* command is used.

Temperature control is achieved with the default Nose-Hoover style thermostat documented in *fix npt*. When this fix is active, only the peculiar velocity of each atom is stored, defined as the velocity relative to the streaming velocity. This is in contrast to *fix nvt/sllod*, which uses a lab-frame velocity, and removes the contribution from the streaming velocity in order to compute the temperature.

Pressure control is achieved using the default Nose-Hoover barostat documented in *fix npt*. There are two ways to control the pressure using this fix. The first method involves using the *ext* keyword along with the *iso* pressure style. With this method, the pressure is controlled by scaling the simulation box isotropically to achieve the average pressure only in the directions specified by *ext*. For example, if the *ext* value is set to *xy*, the average pressure (Pxx+Pyy)/2 will be controlled.

This example command will control the total hydrostatic pressure under uniaxial tension:

```
fix f1 all npt/uef temp 0.7 0.7 0.5 iso 1 1 5 erate -0.5 -0.5 ext xyz
```

This example command will control the average stress in compression directions, which would typically correspond to free surfaces under drawing with uniaxial tension:

```
fix f2 all npt/uef temp 0.7 0.7 0.5 iso 1 1 5 erate -0.5 -0.5 ext xy
```

The second method for pressure control involves setting the normal stresses using the *x*, *y* , and/or *z* keywords. When using this method, the same pressure must be specified via *Pstart* and *Pstop* for all dimensions controlled. Any choice of pressure conditions that would cause LAMMPS to compute a deviatoric stress are not permissible and will result in an error. Additionally, all dimensions with controlled stress must have the same applied strain rate. The *ext* keyword must be set to the default value (*xyz*) when using this method.

For example, the following commands will work:

```
fix f3 all npt/uef temp 0.7 0.7 0.5 x 1 1 5 y 1 1 5 erate -0.5 -0.5
fix f4 all npt/uef temp 0.7 0.7 0.5 z 1 1 5 erate 0.5 0.5
```

The following commands will not work:

```
fix f5 all npt/uef temp 0.7 0.7 0.5 x 1 1 5 z 1 1 5 erate -0.5 -0.5
fix f6 all npt/uef temp 0.7 0.7 0.5 x 1 1 5 z 2 2 5 erate 0.5 0.5
```

These fix computes a temperature and pressure each timestep. To do this, it creates its own computes of style "temp/uef" and "pressure/uef", as if one of these two sets of commands had been issued:

```
compute fix-ID_temp group-ID temp/uef
compute fix-ID_press group-ID pressure/uef fix-ID_temp

compute fix-ID_temp all temp/uef
compute fix-ID_press all pressure/uef fix-ID_temp
```

See the *compute temp/uef* and *compute pressure/uef* commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press".

Restart, fix_modify, output, run start/stop, minimize info:

The fix writes the state of all the thermostat and barostat variables, as well as the cumulative strain applied, to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

Note: It is not necessary to set the *strain* keyword when resuming a run from a restart file. Only for resuming from data files, which do not contain the cumulative applied strain, will this keyword be necessary.

This fix can be used with the *fix_modify* *temp* and *press* options. The temperature and pressure computes used must be of type *temp/uef* and *pressure/uef*.

This fix computes the same global scalar and vector quantities as *fix npt*.

The fix is not invoked during *energy minimization*.

16.110.4 Restrictions

This fix is part of the USER-UEF package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Due to requirements of the boundary conditions, when the *strain* keyword is set to zero (or unset), the initial simulation box must be cubic and have style triclinic. If the box is initially of type ortho, use *change_box* before invoking the fix.

Note: When resuming from restart files, you may need to use *box tilt large* since lammps has internal criteria from lattice reduction that are not the same as the criteria in the numerical lattice reduction algorithm.

16.110.5 Related commands

fix nvt, *fix nvt/sllod*, *compute temp/uef*, *compute pressure/uef*, *dump cfg/uef*

16.110.6 Default

The default keyword values specific to this fix are exy = xyz, strain = 0 0. The remaining defaults are the same as for *fix npt*_fix_nh.html except tchain = 1. The reason for this change is given in *fix nvt/sllod*.

(Dobson) Dobson, J Chem Phys, 141, 184103 (2014).

(Hunt) Hunt, Mol Simul, 42, 347 (2016).

(Semaev) Semaev, Cryptography and Lattices, 181 (2001).

(Evans and Morriss) Evans and Morriss, Phys Rev A, 30, 1528 (1984).

(Nicholson and Rutledge) Nicholson and Rutledge, J Chem Phys, 145, 244903 (2016).

16.111 fix nph/asphere command

16.112 fix nph/asphere/omp command

16.112.1 Syntax

```
fix ID group-ID nph/asphere args keyword value ...
```

- ID, group-ID are documented in *fix* command
- nph/asphere = style name of this fix command
- additional barostat related keyword/value pairs from the *fix nph* command can be appended

16.112.2 Examples

```
fix 1 all nph/asphere iso 0.0 0.0 1000.0
fix 2 all nph/asphere x 5.0 5.0 1000.0
fix 2 all nph/asphere x 5.0 5.0 1000.0 drag 0.2
fix 2 water nph/asphere aniso 0.0 0.0 1000.0 dilate partial
```

16.112.3 Description

Perform constant NPH integration to update position, velocity, orientation, and angular velocity each timestep for aspherical or ellipsoidal particles in the group using a Nose/Hoover pressure barostat. P is pressure; H is enthalpy. This creates a system trajectory consistent with the isenthalpic ensemble.

This fix differs from the *fix nph* command, which assumes point particles and only updates their position and velocity.

Additional parameters affecting the barostat are specified by keywords and values documented with the *fix nph* command. See, for example, discussion of the *aniso*, and *dilate* keywords.

The particles in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the NPH integration.

Regardless of what particles are in the fix group, a global pressure is computed for all particles. Similarly, when the size of the simulation box is changed, all particles are re-scaled to new positions, unless the keyword *dilate* is specified with a value of *partial*, in which case only the particles in the fix group are re-scaled. The latter can be useful for leaving the coordinates of particles in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp/asphere" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp all temp/asphere
compute fix-ID_press all pressure fix-ID_temp
```

See the *compute temp/asphere* and *compute pressure* commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the *compute_modify* command or print this temperature or pressure during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover barostat to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify* *temp* and *press* options are supported by this fix. You can use them to assign a *compute* you have defined to this fix which will be used in its thermostatting or barostatting procedure. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The *fix_modify* *energy* option is supported by this fix to add the energy change induced by Nose/Hoover barostatting to the system's potential energy as part of *thermodynamic output*.

This fix computes the same global scalar and global vector of quantities as does the *fix nph* command.

This fix can ramp its target pressure over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.112.4 Restrictions

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix requires that atoms store torque and angular momentum and a quaternion as defined by the *atom_style ellipsoid* command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or spherical as defined by their shape attribute.

16.112.5 Related commands

fix nph, *fix nve_asphere*, *fix nvt_asphere*, *fix npt_asphere*, *fix_modify*

Default: none

16.113 fix nph/body command

16.113.1 Syntax

```
fix ID group-ID nph/body args keyword value ...
```

- ID, group-ID are documented in *fix* command
- nph/body = style name of this fix command
- additional barostat related keyword/value pairs from the *fix nph* command can be appended

16.113.2 Examples

```
fix 1 all nph/body iso 0.0 0.0 1000.0
fix 2 all nph/body x 5.0 5.0 1000.0
fix 2 all nph/body x 5.0 5.0 1000.0 drag 0.2
fix 2 water nph/body aniso 0.0 0.0 1000.0 dilate partial
```

16.113.3 Description

Perform constant NPH integration to update position, velocity, orientation, and angular velocity each timestep for body particles in the group using a Nose/Hoover pressure barostat. P is pressure; H is enthalpy. This creates a system trajectory consistent with the isenthalpic ensemble.

This fix differs from the *fix nph* command, which assumes point particles and only updates their position and velocity.

Additional parameters affecting the barostat are specified by keywords and values documented with the *fix nph* command. See, for example, discussion of the *aniso*, and *dilate* keywords.

The particles in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the NPH integration.

Regardless of what particles are in the fix group, a global pressure is computed for all particles. Similarly, when the size of the simulation box is changed, all particles are re-scaled to new positions, unless the keyword *dilate* is specified with a value of *partial*, in which case only the particles in the fix group are re-scaled. The latter can be useful for leaving the coordinates of particles in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp/body" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp all temp/body
compute fix-ID_press all pressure fix-ID_temp
```

See the *compute temp/body* and *compute pressure* commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the *compute_modify* command or print this temperature or pressure during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover barostat to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify* *temp* and *press* options are supported by this fix. You can use them to assign a *compute* you have defined to this fix which will be used in its thermostatting or barostatting procedure. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The *fix_modify* *energy* option is supported by this fix to add the energy change induced by Nose/Hoover barostatting to the system's potential energy as part of *thermodynamic output*.

This fix computes the same global scalar and global vector of quantities as does the *fix nph* command.

This fix can ramp its target pressure over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.113.4 Restrictions

This fix is part of the BODY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix requires that atoms store torque and angular momentum and a quaternion as defined by the *atom_style body* command.

16.113.5 Related commands

fix nph, *fix nve_body*, *fix nvt_body*, *fix npt_body*, *fix_modify*

Default: none

16.114 fix nph/sphere command

16.115 fix nph/sphere/omp command

16.115.1 Syntax

```
fix ID group-ID nph/sphere args keyword value ...
```

- ID, group-ID are documented in *fix* command
- nph/sphere = style name of this fix command
- keyword = *disc*

  disc value = none = treat particles as 2d discs, not spheres
- additional barostat related keyword/value pairs from the *fix nph* command can be appended

16.115.2 Examples

```
fix 1 all nph/sphere iso 0.0 0.0 1000.0
fix 2 all nph/sphere x 5.0 5.0 1000.0
fix 2 all nph/sphere x 5.0 5.0 1000.0 disc
fix 2 all nph/sphere x 5.0 5.0 1000.0 drag 0.2
fix 2 water nph/sphere aniso 0.0 0.0 1000.0 dilate partial
```

16.115.3 Description

Perform constant NPH integration to update position, velocity, and angular velocity each timestep for finite-size spherical particles in the group using a Nose/Hoover pressure barostat. P is pressure; H is enthalpy. This creates a system trajectory consistent with the isenthalpic ensemble.

This fix differs from the *fix nph* command, which assumes point particles and only updates their position and velocity.

If the *disc* keyword is used, then each particle is treated as a 2d disc (circle) instead of as a sphere. This is only possible for 2d simulations, as defined by the *dimension* keyword. The only difference between discs and spheres in this context is their moment of inertia, as used in the time integration.

Additional parameters affecting the barostat are specified by keywords and values documented with the *fix nph* command. See, for example, discussion of the *aniso*, and *dilate* keywords.

The particles in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the NPH integration.

Regardless of what particles are in the fix group, a global pressure is computed for all particles. Similarly, when the size of the simulation box is changed, all particles are re-scaled to new positions, unless the keyword *dilate* is specified with a value of *partial*, in which case only the particles in the fix group are re-scaled. The latter can be useful for leaving the coordinates of particles in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp/sphere" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp all temp/sphere
compute fix-ID_press all pressure fix-ID_temp
```

See the *compute temp/sphere* and *compute pressure* commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the *compute_modify* command or print this temperature or pressure during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover barostat to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify* *temp* and *press* options are supported by this fix. You can use them to assign a *compute* you have defined to this fix which will be used in its thermostatting or barostatting procedure. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The *fix_modify* *energy* option is supported by this fix to add the energy change induced by Nose/Hoover barostatting to the system's potential energy as part of *thermodynamic output*.

This fix computes the same global scalar and global vector of quantities as does the *fix nph* command.

This fix can ramp its target pressure over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.115.4 Restrictions

This fix requires that atoms store torque and angular velocity (omega) and a radius as defined by the *atom_style sphere* command.

All particles in the group must be finite-size spheres. They cannot be point particles.

Use of the *disc* keyword is only allowed for 2d simulations, as defined by the *dimension* keyword.

16.115.5 Related commands

fix nph, *fix nve_sphere*, *fix nvt_sphere*, *fix npt_sphere*, *fix_modify*

Default: none

16.116 fix nphug command

16.117 fix nphug/omp command

16.117.1 Syntax

```
fix ID group-ID nphug keyword value ...
```

- ID, group-ID are documented in *fix* command

  one or more keyword value pairs may be appended
  keyword = *temp* or *iso* or *aniso* or *tri* or *x* or *y* or *z* or *couple* or *tchain* or *pchain* or *mtk* or *tloop* or *ploop* or *nreset* or *drag* or *dilate* or *scaleyz* or *scalexz* or *scalexy*

```
  temp values = Value1 Value2 Tdamp
    Value1, Value2 = Nose-Hoover target temperatures, ignored by␣
↪Hugoniostat
    Tdamp = temperature damping parameter (time units)
  iso or aniso or tri values = Pstart Pstop Pdamp
    Pstart,Pstop = scalar external pressures, must be equal (pressure␣
↪units)
    Pdamp = pressure damping parameter (time units)
  x or y or z or xy or yz or xz values = Pstart Pstop Pdamp
    Pstart,Pstop = external stress tensor components, must be equal␣
↪(pressure units)
    Pdamp = stress damping parameter (time units)
  couple = none or xyz or xy or yz or xz
  tchain value = length of thermostat chain (1 = single thermostat)
  pchain values = length of thermostat chain on barostat (0 = no␣
↪thermostat)
  mtk value = yes or no = add in MTK adjustment term or not
  tloop value = number of sub-cycles to perform on thermostat
  ploop value = number of sub-cycles to perform on barostat thermostat
  nreset value = reset reference cell every this many timesteps
  drag value = drag factor added to barostat/thermostat (0.0 = no drag)
  dilate value = all or partial
  scaleyz value = yes or no = scale yz with lz
  scalexz value = yes or no = scale xz with lz
  scalexy value = yes or no = scale xy with ly
```

16.117.2 Examples

```
fix myhug all nphug temp 1.0 1.0 10.0 z 40.0 40.0 70.0
fix myhug all nphug temp 1.0 1.0 10.0 iso 40.0 40.0 70.0 drag 200.0 tchain 1 pchain 0
```

16.117.3 Description

This command is a variant of the Nose-Hoover *fix npt* fix style. It performs time integration of the Hugoniostat equations of motion developed by Ravelo et al. *(Ravelo)*. These equations compress the system to a state with average axial stress or pressure equal to the specified target value and that satisfies the Rankine-Hugoniot (RH) jump conditions for steady shocks.

The compression can be performed either hydrostatically (using keyword *iso*, *aniso*, or *tri*) or uniaxially (using keywords *x*, *y*, or *z*). In the hydrostatic case, the cell dimensions change dynamically so that the average axial stress in all three directions converges towards the specified target value. In the uniaxial case, the chosen cell dimension changes dynamically so that the average axial stress in that direction converges towards the target value. The other two cell dimensions are kept fixed (zero lateral strain).

This leads to the following additional restrictions on the keywords:

- One and only one of the following keywords should be used: *iso*, *aniso*, *tri*, *x*, *y*, *z*
- The specified initial and final target pressures must be the same.
- The keywords *xy*, *xz*, *yz* may not be used.
- The only admissible value for the couple keyword is *xyz*, which has the same effect as keyword *iso*

- The *temp* keyword must be used to specify the time constant for kinetic energy relaxation, but initial and final target temperature values are ignored.

Essentially, a Hugoniostat simulation is an NPT simulation in which the user-specified target temperature is replaced with a time-dependent target temperature Tt obtained from the following equation:

$$T_t - T = \frac{\left(\frac{1}{2}\left(P + P_0\right)\left(V_0 - V\right) + E_0 - E\right)}{N_{dof} k_B} = \Delta$$

where T and T_t are the instantaneous and target temperatures, P and P_0 are the instantaneous and reference pressures or axial stresses, depending on whether hydrostatic or uniaxial compression is being performed, V and V_0 are the instantaneous and reference volumes, E and E_0 are the instantaneous and reference internal energy (potential plus kinetic), N_{dof} is the number of degrees of freedom used in the definition of temperature, and k_B is the Boltzmann constant. Δ is the negative deviation of the instantaneous temperature from the target temperature. When the system reaches a stable equilibrium, the value of Δ should fluctuate about zero.

The values of E_0, V_0, and P_0 are the instantaneous values at the start of the simulation. These can be overridden using the fix_modify keywords *e0*, *v0*, and *p0* described below.

Note: Unlike the *fix temp/berendsen* command which performs thermostatting but NO time integration, this fix performs thermostatting/barostatting AND time integration. Thus you should not use any other time integration fix, such as *fix nve* on atoms to which this fix is applied. Likewise, this fix should not be used on atoms that have their temperature controlled by another fix - e.g. by *fix langevin* or *fix temp/rescale* commands.

This fix computes a temperature and pressure at each timestep. To do this, the fix creates its own computes of style "temp" and "pressure", as if one of these two sets of commands had been issued:

```
compute fix-ID_temp group-ID temp
compute fix-ID_press group-ID pressure fix-ID_temp

compute fix-ID_temp all temp
compute fix-ID_press all pressure fix-ID_temp
```

See the *compute temp* and *compute pressure* commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press". The group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the *compute_modify* command or print this temperature or pressure during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the values of E_0, V_0, and P_0, as well as the state of all the thermostat and barostat variables to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify* *e0*, *v0* and *p0* keywords can be used to define the values of E_0, V_0, and P_0. Note the the values for *e0* and *v0* are extensive, and so must correspond to the total energy and volume of the entire system, not energy and volume per atom. If any of these quantities are not specified, then the instantaneous value in the system at the start of the simulation is used.

The *fix_modify* *temp* and *press* options are supported by these fixes. You can use them to assign a *compute* you have defined to this fix which will be used in its thermostatting or barostatting procedure, as described above. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The *fix_modify* *energy* option is supported by these fixes to add the energy change induced by Nose/Hoover thermostatting and barostatting to the system's potential energy as part of *thermodynamic output*. Either way, this energy is *not* included in the definition of internal energy E when calculating the value of Delta in the above equation.

These fixes compute a global scalar and a global vector of quantities, which can be accessed by various *output commands*. The scalar value calculated by these fixes is "extensive"; the vector values are "intensive".

The scalar is the cumulative energy change due to the fix.

The vector stores three quantities unique to this fix (Δ, Us, and up), followed by all the internal Nose/Hoover thermostat and barostat variables defined for *fix npt*. Delta is the deviation of the temperature from the target temperature, given by the above equation. Us and up are the shock and particle velocity corresponding to a steady shock calculated from the RH conditions. They have units of distance/time.

16.117.4 Restrictions

This fix style is part of the SHOCK package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

All the usual restrictions for *fix npt* apply, plus the additional ones mentioned above.

16.117.5 Related commands

fix msst, *fix npt*, *fix_modify*

16.117.6 Default

The keyword defaults are the same as those for *fix npt*

(Ravelo) Ravelo, Holian, Germann and Lomdahl, Phys Rev B, 70, 014103 (2004).

16.118 fix npt/asphere command

16.119 fix npt/asphere/omp command

16.119.1 Syntax

```
fix ID group-ID npt/asphere keyword value ...
```

- ID, group-ID are documented in *fix* command
- npt/asphere = style name of this fix command
- additional thermostat and barostat related keyword/value pairs from the *fix npt* command can be appended

16.119.2 Examples

```
fix 1 all npt/asphere temp 300.0 300.0 100.0 iso 0.0 0.0 1000.0
fix 2 all npt/asphere temp 300.0 300.0 100.0 x 5.0 5.0 1000.0
fix 2 all npt/asphere temp 300.0 300.0 100.0 x 5.0 5.0 1000.0 drag 0.2
fix 2 water npt/asphere temp 300.0 300.0 100.0 aniso 0.0 0.0 1000.0 dilate partial
```

16.119.3 Description

Perform constant NPT integration to update position, velocity, orientation, and angular velocity each timestep for aspherical or ellipsoidal particles in the group using a Nose/Hoover temperature thermostat and Nose/Hoover pressure barostat. P is pressure; T is temperature. This creates a system trajectory consistent with the isothermal-isobaric ensemble.

This fix differs from the *fix npt* command, which assumes point particles and only updates their position and velocity.

The thermostat is applied to both the translational and rotational degrees of freedom for the aspherical particles, assuming a compute is used which calculates a temperature that includes the rotational degrees of freedom (see below). The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

Additional parameters affecting the thermostat and barostat are specified by keywords and values documented with the *fix npt* command. See, for example, discussion of the *temp*, *iso*, *aniso*, and *dilate* keywords.

The particles in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the NPT integration.

Regardless of what particles are in the fix group, a global pressure is computed for all particles. Similarly, when the size of the simulation box is changed, all particles are re-scaled to new positions, unless the keyword *dilate* is specified with a value of *partial*, in which case only the particles in the fix group are re-scaled. The latter can be useful for leaving the coordinates of particles in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp/asphere" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp all temp/asphere
compute fix-ID_press all pressure fix-ID_temp
```

See the *compute temp/asphere* and *compute pressure* commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the *compute_modify* command or print this temperature or pressure during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with *compute commands* that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the *fix_modify* command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual *compute commands* to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover thermostat and barostat to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify temp* and *press* options are supported by this fix. You can use them to assign a *compute* you have defined to this fix which will be used in its thermostatting or barostatting procedure. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The *fix_modify energy* option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting and barostatting to the system's potential energy as part of *thermodynamic output*.

This fix computes the same global scalar and global vector of quantities as does the *fix npt* command.

This fix can ramp its target temperature and pressure over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.119.4 Restrictions

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix requires that atoms store torque and angular momentum and a quaternion as defined by the *atom_style ellipsoid* command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or spherical as defined by their shape attribute.

16.119.5 Related commands

fix npt, *fix nve_asphere*, *fix nvt_asphere*, *fix_modify*

Default: none

16.120 fix npt/body command

16.120.1 Syntax

```
fix ID group-ID npt/body keyword value ...
```

- ID, group-ID are documented in *fix* command
- npt/body = style name of this fix command
- additional thermostat and barostat related keyword/value pairs from the *fix npt* command can be appended

16.120.2 Examples

```
fix 1 all npt/body temp 300.0 300.0 100.0 iso 0.0 0.0 1000.0
fix 2 all npt/body temp 300.0 300.0 100.0 x 5.0 5.0 1000.0
fix 2 all npt/body temp 300.0 300.0 100.0 x 5.0 5.0 1000.0 drag 0.2
fix 2 water npt/body temp 300.0 300.0 100.0 aniso 0.0 0.0 1000.0 dilate partial
```

16.120.3 Description

Perform constant NPT integration to update position, velocity, orientation, and angular velocity each timestep for body particles in the group using a Nose/Hoover temperature thermostat and Nose/Hoover pressure barostat. P is pressure; T is temperature. This creates a system trajectory consistent with the isothermal-isobaric ensemble.

This fix differs from the *fix npt* command, which assumes point particles and only updates their position and velocity.

The thermostat is applied to both the translational and rotational degrees of freedom for the body particles, assuming a compute is used which calculates a temperature that includes the rotational degrees of freedom (see below). The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

Additional parameters affecting the thermostat and barostat are specified by keywords and values documented with the *fix npt* command. See, for example, discussion of the *temp*, *iso*, *aniso*, and *dilate* keywords.

The particles in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the NPT integration.

Regardless of what particles are in the fix group, a global pressure is computed for all particles. Similarly, when the size of the simulation box is changed, all particles are re-scaled to new positions, unless the keyword *dilate* is specified with a value of *partial*, in which case only the particles in the fix group are re-scaled. The latter can be useful for leaving the coordinates of particles in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp/body" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp all temp/body
compute fix-ID_press all pressure fix-ID_temp
```

See the *compute temp/body* and *compute pressure* commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the *compute_modify* command or print this temperature or pressure during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with *compute commands* that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the *fix_modify* command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual *compute commands* to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover thermostat and barostat to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify temp* and *press* options are supported by this fix. You can use them to assign a *compute* you have defined to this fix which will be used in its thermostatting or barostatting procedure. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The *fix_modify energy* option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting and barostatting to the system's potential energy as part of *thermodynamic output*.

This fix computes the same global scalar and global vector of quantities as does the *fix npt* command.

This fix can ramp its target temperature and pressure over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.120.4 Restrictions

This fix is part of the BODY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix requires that atoms store torque and angular momentum and a quaternion as defined by the *atom_style body* command.

16.120.5 Related commands

fix npt, *fix nve_body*, *fix nvt_body*, *fix_modify*

Default: none

16.121 fix npt/cauchy command

16.121.1 Syntax

```
fix ID group-ID style_name keyword value ...
```

- ID, group-ID are documented in *fix* command
- style_name = *npt/cauchy*
- one or more keyword/value pairs may be appended
- keyword = *temp* or *iso* or *aniso* or *tri* or *x* or *y* or *z* or *xy* or *yz* or *xz* or *couple* or *tchain* or *pchain* or *mtk* or *tloop* or *ploop* or *nreset* or *drag* or *dilate* or *scalexy* or *scaleyz* or *scalexz* or *flip* or *fixedpoint* or *update*

```
temp values = Tstart Tstop Tdamp
  Tstart,Tstop = external temperature at start/end of run
  Tdamp = temperature damping parameter (time units)
iso or aniso or tri values = Pstart Pstop Pdamp
  Pstart,Pstop = scalar external pressure at start/end of run (pressure␣
↪units)
  Pdamp = pressure damping parameter (time units)
x or y or z or xy or yz or xz values = Pstart Pstop Pdamp
  Pstart,Pstop = external stress tensor component at start/end of run␣
↪(pressure units)
  Pdamp = stress damping parameter (time units)
couple = none or xyz or xy or yz or xz
tchain value = N
  N = length of thermostat chain (1 = single thermostat)
pchain values = N
  N length of thermostat chain on barostat (0 = no thermostat)
```

```
mtk value = yes or no = add in MTK adjustment term or not
tloop value = M
  M = number of sub-cycles to perform on thermostat
ploop value = M
  M = number of sub-cycles to perform on barostat thermostat
nreset value = reset reference cell every this many timesteps
drag value = Df
  Df = drag factor added to barostat/thermostat (0.0 = no drag)
dilate value = dilate-group-ID
  dilate-group-ID = only dilate atoms in this group due to barostat␣
↪volume changes
scalexy value = yes or no = scale xy with ly
scaleyz value = yes or no = scale yz with lz
scalexz value = yes or no = scale xz with lz
flip value = yes or no = allow or disallow box flips when it becomes␣
↪highly skewed
cauchystat cauchystat values = alpha continue
  alpha = strength of Cauchy stress control parameter
  continue = yes or no = whether of not to continue from a previous run
fixedpoint values = x y z
  x,y,z = perform barostat dilation/contraction around this point␣
↪(distance units)
```

16.121.2 Examples

fix 1 water npt/cauchy temp 300.0 300.0 100.0 iso 0.0 0.0 1000.0

16.121.3 Description

This command performs time integration on Nose-Hoover style non-Hamiltonian equations of motion which are designed to generate positions and velocities sampled from the isothermal-isobaric (npt) ensembles. This updates the position and velocity for atoms in the group each timestep and the box dimensions.

The thermostatting and barostatting is achieved by adding some dynamic variables which are coupled to the particle velocities (thermostatting) and simulation domain dimensions (barostatting). In addition to basic thermostatting and barostatting, this fix can also create a chain of thermostats coupled to the particle thermostat, and another chain of thermostats coupled to the barostat variables. The barostat can be coupled to the overall box volume, or to individual dimensions, including the *xy*, *xz* and *yz* tilt dimensions. The external pressure of the barostat can be specified as either a scalar pressure (isobaric ensemble) or as components of a symmetric stress tensor (constant stress ensemble). When used correctly, the time-averaged temperature and stress tensor of the particles will match the target values specified by Tstart/Tstop and Pstart/Pstop.

The equations of motion used are those of Shinoda et al in *(Shinoda)*, which combine the hydrostatic equations of Martyna, Tobias and Klein in *(Martyna)* with the strain energy proposed by Parrinello and Rahman in *(Parrinello)*. The time integration schemes closely follow the time-reversible measure-preserving Verlet and rRESPA integrators derived by Tuckerman et al in *(Tuckerman)*.

The thermostat parameters are specified using the *temp* keyword. Other thermostat-related keywords are *tchain*, *tloop* and *drag*, which are discussed below.

The thermostat is applied to only the translational degrees of freedom for the particles. The translational degrees of freedom can also have a bias velocity removed before thermostatting takes place; see the description below. The desired temperature at each timestep is a ramped value during the run from *Tstart* to *Tstop*. The *Tdamp* parameter is

specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 10.0 means to relax the temperature in a timespan of (roughly) 10 time units (e.g. tau or fmsec or psec - see the *units* command). The atoms in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the integration.

Note: A Nose-Hoover thermostat will not work well for arbitrary values of *Tdamp*. If *Tdamp* is too small, the temperature can fluctuate wildly; if it is too large, the temperature will take a very long time to equilibrate. A good choice for many models is a *Tdamp* of around 100 timesteps. Note that this is NOT the same as 100 time units for most *units* settings.

The barostat parameters are specified using one or more of the *iso*, *aniso*, *tri*, *x*, *y*, *z*, *xy*, *xz*, *yz*, and *couple* keywords. These keywords give you the ability to specify all 6 components of an external stress tensor, and to couple various of these components together so that the dimensions they represent are varied together during a constant-pressure simulation.

Other barostat-related keywords are *pchain*, *mtk*, *ploop*, *nreset*, *drag*, and *dilate*, which are discussed below.

Orthogonal simulation boxes have 3 adjustable dimensions (x,y,z). Triclinic (non-orthogonal) simulation boxes have 6 adjustable dimensions (x,y,z,xy,xz,yz). The *create_box*, *read data*, and *read_restart* commands specify whether the simulation box is orthogonal or non-orthogonal (triclinic) and explain the meaning of the xy,xz,yz tilt factors.

The target pressures for each of the 6 components of the stress tensor can be specified independently via the *x*, *y*, *z*, *xy*, *xz*, *yz* keywords, which correspond to the 6 simulation box dimensions. For each component, the external pressure or tensor component at each timestep is a ramped value during the run from *Pstart* to *Pstop*. If a target pressure is specified for a component, then the corresponding box dimension will change during a simulation. For example, if the *y* keyword is used, the y-box length will change. If the *xy* keyword is used, the xy tilt factor will change. A box dimension will not change if that component is not specified, although you have the option to change that dimension via the *fix deform* command.

Note that in order to use the *xy*, *xz*, or *yz* keywords, the simulation box must be triclinic, even if its initial tilt factors are 0.0.

For all barostat keywords, the *Pdamp* parameter operates like the *Tdamp* parameter, determining the time scale on which pressure is relaxed. For example, a value of 10.0 means to relax the pressure in a timespan of (roughly) 10 time units (e.g. tau or fmsec or psec - see the *units* command).

Note: A Nose-Hoover barostat will not work well for arbitrary values of *Pdamp*. If *Pdamp* is too small, the pressure and volume can fluctuate wildly; if it is too large, the pressure will take a very long time to equilibrate. A good choice for many models is a *Pdamp* of around 1000 timesteps. However, note that *Pdamp* is specified in time units, and that timesteps are NOT the same as time units for most *units* settings.

Regardless of what atoms are in the fix group (the only atoms which are time integrated), a global pressure or stress tensor is computed for all atoms. Similarly, when the size of the simulation box is changed, all atoms are re-scaled to new positions, unless the keyword *dilate* is specified with a *dilate-group-ID* for a group that represents a subset of the atoms. This can be useful, for example, to leave the coordinates of atoms in a solid substrate unchanged and controlling the pressure of a surrounding fluid. This option should be used with care, since it can be unphysical to dilate some atoms and not others, because it can introduce large, instantaneous displacements between a pair of atoms (one dilated, one not) that are far from the dilation origin. Also note that for atoms not in the fix group, a separate time integration fix like *fix nve* or *fix nvt* can be used on them, independent of whether they are dilated or not.

The *couple* keyword allows two or three of the diagonal components of the pressure tensor to be "coupled" together. The value specified with the keyword determines which are coupled. For example, *xz* means the *Pxx* and *Pzz* components of the stress tensor are coupled. *Xyz* means all 3 diagonal components are coupled. Coupling means two things:

the instantaneous stress will be computed as an average of the corresponding diagonal components, and the coupled box dimensions will be changed together in lockstep, meaning coupled dimensions will be dilated or contracted by the same percentage every timestep. The *Pstart*, *Pstop*, *Pdamp* parameters for any coupled dimensions must be identical. *Couple xyz* can be used for a 2d simulation; the *z* dimension is simply ignored.

The *iso*, *aniso*, and *tri* keywords are simply shortcuts that are equivalent to specifying several other keywords together.

The keyword *iso* means couple all 3 diagonal components together when pressure is computed (hydrostatic pressure), and dilate/contract the dimensions together. Using "iso Pstart Pstop Pdamp" is the same as specifying these 4 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
couple xyz
```

The keyword *aniso* means *x*, *y*, and *z* dimensions are controlled independently using the *Pxx*, *Pyy*, and *Pzz* components of the stress tensor as the driving forces, and the specified scalar external pressure. Using "aniso Pstart Pstop Pdamp" is the same as specifying these 4 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
couple none
```

The keyword *tri* means *x*, *y*, *z*, *xy*, *xz*, and *yz* dimensions are controlled independently using their individual stress components as the driving forces, and the specified scalar pressure as the external normal stress. Using "tri Pstart Pstop Pdamp" is the same as specifying these 7 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
xy 0.0 0.0 Pdamp
yz 0.0 0.0 Pdamp
xz 0.0 0.0 Pdamp
couple none
```

In some cases (e.g. for solids) the pressure (volume) and/or temperature of the system can oscillate undesirably when a Nose/Hoover barostat and thermostat is applied. The optional *drag* keyword will damp these oscillations, although it alters the Nose/Hoover equations. A value of 0.0 (no drag) leaves the Nose/Hoover formalism unchanged. A non-zero value adds a drag term; the larger the value specified, the greater the damping effect. Performing a short run and monitoring the pressure and temperature is the best way to determine if the drag term is working. Typically a value between 0.2 to 2.0 is sufficient to damp oscillations after a few periods. Note that use of the drag keyword will interfere with energy conservation and will also change the distribution of positions and velocities so that they do not correspond to the nominal NVT, NPT, or NPH ensembles.

An alternative way to control initial oscillations is to use chain thermostats. The keyword *tchain* determines the number of thermostats in the particle thermostat. A value of 1 corresponds to the original Nose-Hoover thermostat. The keyword *pchain* specifies the number of thermostats in the chain thermostatting the barostat degrees of freedom. A value of 0 corresponds to no thermostatting of the barostat variables.

The *mtk* keyword controls whether or not the correction terms due to Martyna, Tuckerman, and Klein are included in the equations of motion *(Martyna)*. Specifying *no* reproduces the original Hoover barostat, whose volume probability distribution function differs from the true NPT and NPH ensembles by a factor of 1/V. Hence using *yes* is more correct, but in many cases the difference is negligible.

The keyword *tloop* can be used to improve the accuracy of integration scheme at little extra cost. The initial and final updates of the thermostat variables are broken up into *tloop* sub-steps, each of length *dt*/*tloop*. This corresponds to using a first-order Suzuki-Yoshida scheme *(Tuckerman)*. The keyword *ploop* does the same thing for the barostat thermostat.

The keyword *nreset* controls how often the reference dimensions used to define the strain energy are reset. If this keyword is not used, or is given a value of zero, then the reference dimensions are set to those of the initial simulation domain and are never changed. If the simulation domain changes significantly during the simulation, then the final average pressure tensor will differ significantly from the specified values of the external stress tensor. A value of *nstep* means that every *nstep* timesteps, the reference dimensions are set to those of the current simulation domain.

The *scaleyz*, *scalexz*, and *scalexy* keywords control whether or not the corresponding tilt factors are scaled with the associated box dimensions when barostatting triclinic periodic cells. The default values *yes* will turn on scaling, which corresponds to adjusting the linear dimensions of the cell while preserving its shape. Choosing *no* ensures that the tilt factors are not scaled with the box dimensions. See below for restrictions and default values in different situations. In older versions of LAMMPS, scaling of tilt factors was not performed. The old behavior can be recovered by setting all three scale keywords to *no*.

The *flip* keyword allows the tilt factors for a triclinic box to exceed half the distance of the parallel box length, as discussed below. If the *flip* value is set to *yes*, the bound is enforced by flipping the box when it is exceeded. If the *flip* value is set to *no*, the tilt will continue to change without flipping. Note that if applied stress induces large deformations (e.g. in a liquid), this means the box shape can tilt dramatically and LAMMPS will run less efficiently, due to the large volume of communication needed to acquire ghost atoms around a processor's irregular-shaped sub-domain. For extreme values of tilt, LAMMPS may also lose atoms and generate an error.

The *fixedpoint* keyword specifies the fixed point for barostat volume changes. By default, it is the center of the box. Whatever point is chosen will not move during the simulation. For example, if the lower periodic boundaries pass through (0,0,0), and this point is provided to *fixedpoint*, then the lower periodic boundaries will remain at (0,0,0), while the upper periodic boundaries will move twice as far. In all cases, the particle trajectories are unaffected by the chosen value, except for a time-dependent constant translation of positions.

Note: Using a barostat coupled to tilt dimensions *xy*, *xz*, *yz* can sometimes result in arbitrarily large values of the tilt dimensions, i.e. a dramatically deformed simulation box. LAMMPS allows the tilt factors to grow a small amount beyond the normal limit of half the box length (0.6 times the box length), and then performs a box "flip" to an equivalent periodic cell. See the discussion of the *flip* keyword above, to allow this bound to be exceeded, if desired.

The flip operation is described in more detail in the doc page for *fix deform*. Both the barostat dynamics and the atom trajectories are unaffected by this operation. However, if a tilt factor is incremented by a large amount (1.5 times the box length) on a single timestep, LAMMPS can not accommodate this event and will terminate the simulation with an error. This error typically indicates that there is something badly wrong with how the simulation was constructed, such as specifying values of *Pstart* that are too far from the current stress value, or specifying a timestep that is too large. Triclinic barostatting should be used with care. This also is true for other barostat styles, although they tend to be more forgiving of insults. In particular, it is important to recognize that equilibrium liquids can not support a shear stress and that equilibrium solids can not support shear stresses that exceed the yield stress.

One exception to this rule is if the 1st dimension in the tilt factor (x for xy) is non-periodic. In that case, the limits on the tilt factor are not enforced, since flipping the box in that dimension does not change the atom positions due to non-periodicity. In this mode, if you tilt the system to extreme angles, the simulation will simply become inefficient due to the highly skewed simulation box.

Note: Unlike the *fix temp/berendsen* command which performs thermostatting but NO time integration, this fix performs thermostatting/barostatting AND time integration. Thus you should not use any other time integration fix,

such as *fix nve* on atoms to which this fix is applied. Likewise, fix npt/cauchy should not normally be used on atoms that also have their temperature controlled by another fix - e.g. by *fix langevin* or *fix temp/rescale* commands.

See the *Howto thermostat* and *Howto barostat* doc pages for a discussion of different ways to compute temperature and perform thermostatting and barostatting.

This fix compute a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp" and "pressure", as if one of these sets of commands had been issued:

```
compute fix-ID_temp all temp
compute fix-ID_press all pressure fix-ID_temp
```

The group for both the new temperature and pressure compute is "all" since pressure is computed for the entire system. See the *compute temp* and *compute pressure* commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press".

Note that these are NOT the computes used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of these fix's temperature or pressure via the *compute_modify* command. Or you can print this temperature or pressure during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Like other fixes that perform thermostatting, fix npt/cauchy can be used with *compute commands* that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the *fix_modify* command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual *compute commands* to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

This fix can be used with either the *verlet* or *respa integrators*. When using this fix with *respa*, LAMMPS uses an integrator constructed according to the following factorization of the Liouville propagator (for two rRESPA levels):

$$
\begin{aligned}
\exp\left(\mathrm{i}L\Delta t\right) =& \hat{E}\exp\left(\mathrm{i}L_{\text{T-baro}}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_{\text{T-part}}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_{\epsilon,2}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_2^{(2)}\frac{\Delta t}{2}\right)\\
&\times\left[\exp\left(\mathrm{i}L_2^{(1)}\frac{\Delta t}{2n}\right)\exp\left(\mathrm{i}L_{\epsilon,1}\frac{\Delta t}{2n}\right)\exp\left(\mathrm{i}L_1\frac{\Delta t}{n}\right)\exp\left(\mathrm{i}L_{\epsilon,1}\frac{\Delta t}{2n}\right)\exp\left(\mathrm{i}L_2^{(1)}\frac{\Delta t}{2n}\right)\right]^n\\
&\times\exp\left(\mathrm{i}L_2^{(2)}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_{\epsilon,2}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_{\text{T-part}}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_{\text{T-baro}}\frac{\Delta t}{2}\right)\\
&+\mathcal{O}\left(\Delta t^3\right)
\end{aligned}
$$

This factorization differs somewhat from that of Tuckerman et al, in that the barostat is only updated at the outermost rRESPA level, whereas Tuckerman's factorization requires splitting the pressure into pieces corresponding to the forces computed at each rRESPA level. In theory, the latter method will exhibit better numerical stability. In practice, because Pdamp is normally chosen to be a large multiple of the outermost rRESPA timestep, the barostat dynamics are not the limiting factor for numerical stability. Both factorizations are time-reversible and can be shown to preserve the phase space measure of the underlying non-Hamiltonian equations of motion.

Note: Under NPT dynamics, for a system with zero initial total linear momentum, the total momentum fluctuates close to zero. It may occasionally undergo brief excursions to non-negligible values, before returning close to zero.

Over long simulations, this has the effect of causing the center-of-mass to undergo a slow random walk. This can be mitigated by resetting the momentum at infrequent intervals using the *fix momentum* command.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of all the thermostat and barostat variables to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify* *temp* and *press* options are supported by this fix. You can use them to assign a *compute* you have defined to this fix which will be used in its thermostatting or barostatting procedure, as described above. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

Note: If both the *temp* and *press* keywords are used in a single thermo_modify command (or in two separate commands), then the order in which the keywords are specified is important. Note that a *pressure compute* defines its own temperature compute as an argument when it is specified. The *temp* keyword will override this (for the pressure compute being used by fix npt), but only if the *temp* keyword comes after the *press* keyword. If the *temp* keyword comes before the *press* keyword, then the new pressure compute specified by the *press* keyword will be unaffected by the *temp* setting.

The *fix_modify* *energy* option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting and barostatting to the system's potential energy as part of *thermodynamic output*.

This fix computes a global scalar and a global vector of quantities, which can be accessed by various *output commands*. The scalar value calculated by this fix is "extensive"; the vector values are "intensive".

The scalar is the cumulative energy change due to the fix.

The vector stores internal Nose/Hoover thermostat and barostat variables. The number and meaning of the vector values depends on which fix is used and the settings for keywords *tchain* and *pchain*, which specify the number of Nose/Hoover chains for the thermostat and barostat. If no thermostatting is done, then *tchain* is 0. If no barostatting is done, then *pchain* is 0. In the following list, "ndof" is 0, 1, 3, or 6, and is the number of degrees of freedom in the barostat. Its value is 0 if no barostat is used, else its value is 6 if any off-diagonal stress tensor component is barostatted, else its value is 1 if *couple xyz* is used or *couple xy* for a 2d simulation, otherwise its value is 3.

The order of values in the global vector and their meaning is as follows. The notation means there are tchain values for eta, followed by tchain for eta_dot, followed by ndof for omega, etc:

- eta[tchain] = particle thermostat displacements (unitless)
- eta_dot[tchain] = particle thermostat velocities (1/time units)
- omega[ndof] = barostat displacements (unitless)
- omega_dot[ndof] = barostat velocities (1/time units)
- etap[pchain] = barostat thermostat displacements (unitless)
- etap_dot[pchain] = barostat thermostat velocities (1/time units)
- PE_eta[tchain] = potential energy of each particle thermostat displacement (energy units)
- KE_eta_dot[tchain] = kinetic energy of each particle thermostat velocity (energy units)
- PE_omega[ndof] = potential energy of each barostat displacement (energy units)
- KE_omega_dot[ndof] = kinetic energy of each barostat velocity (energy units)

- PE_etap[pchain] = potential energy of each barostat thermostat displacement (energy units)
- KE_etap_dot[pchain] = kinetic energy of each barostat thermostat velocity (energy units)
- PE_strain[1] = scalar strain energy (energy units)

This fix can ramp its external temperature and pressure over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.121.4 Restrictions

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

X, *y*, *z* cannot be barostatted if the associated dimension is not periodic. *Xy*, *xz*, and *yz* can only be barostatted if the simulation domain is triclinic and the 2nd dimension in the keyword (*y* dimension in *xy*) is periodic. *Z*, *xz*, and *yz*, cannot be barostatted for 2D simulations. The *create_box*, *read data*, and *read_restart* commands specify whether the simulation box is orthogonal or non-orthogonal (triclinic) and explain the meaning of the xy,xz,yz tilt factors.

For the *temp* keyword, the final Tstop cannot be 0.0 since it would make the external T = 0.0 at some timestep during the simulation which is not allowed in the Nose/Hoover formulation.

The *scaleyz yes* and *scalexz yes* keyword/value pairs can not be used for 2D simulations. *scaleyz yes*, *scalexz yes*, and *scalexy yes* options can only be used if the 2nd dimension in the keyword is periodic, and if the tilt factor is not coupled to the barostat via keywords *tri*, *yz*, *xz*, and *xy*.

Without the *cauchystat* keyword, the barostat algorithm controls the Second-Piola Kirchhoff stress, which is a stress measure referred to the unmodified (initial) simulation box. If the box deforms substantially during the equilibration, the difference between the set values and the final true (Cauchy) stresses can be considerable.

The *cauchystat* keyword modifies the barostat as per Miller et al. (Miller)_"#nc-Miller" so that the Cauchy stress is controlled. *alpha* is the non-dimensional parameter, typically set to 0.001 or 0.01 that determines how aggressively the algorithm drives the system towards the set Cauchy stresses. Larger values of *alpha* will modify the system more quickly, but can lead to instabilities. Smaller values will lead to longer convergence time. Since *alpha* also influences how much the stress fluctuations deviate from the equilibrium fluctuations, it should be set as small as possible.

A *continue* value of *yes* indicates that the fix is subsequent to a previous run with the npt/cauchy fix, and the intention is to continue from the converged stress state at the end of the previous run. This may be required, for example, when implementing a multi-step loading/unloading sequence over several fixes.

Setting *alpha* to zero is not permitted. To "turn off" the cauchystat control and thus restore the equilibrium stress fluctuations, two subsequent fixes should be used. In the first, the cauchystat flag is used and the simulation box equilibrates to the correct shape for the desired stresses. In the second, the *fix* statement is identical except that the *cauchystat* keyword is removed (along with related *alpha* and *continue* values). This restores the original Parrinello-Rahman algorithm, but now with the correct simulation box shape from the first fix.

This fix can be used with dynamic groups as defined by the *group* command. Likewise it can be used with groups to which atoms are added or deleted over time, e.g. a deposition simulation. However, the conservation properties of the thermostat and barostat are defined for systems with a static set of atoms. You may observe odd behavior if the atoms in a group vary dramatically over time or the atom count becomes very small.

16.121.5 Related commands

fix nve, *fix_modify*, *run_style*

16.121.6 Default

The keyword defaults are tchain = 3, pchain = 3, mtk = yes, tloop = ploop = 1, nreset = 0, drag = 0.0, dilate = all, couple = none, cauchystat = no, scaleyz = scalexz = scalexy = yes if periodic in 2nd dimension and not coupled to barostat, otherwise no.

(Martyna) Martyna, Tobias and Klein, J Chem Phys, 101, 4177 (1994).

(Parrinello) Parrinello and Rahman, J Appl Phys, 52, 7182 (1981).

(Tuckerman) Tuckerman, Alejandre, Lopez-Rendon, Jochim, and Martyna, J Phys A: Math Gen, 39, 5629 (2006).

(Shinoda) Shinoda, Shiga, and Mikami, Phys Rev B, 69, 134103 (2004).

(Miller) Miller, Tadmor, Gibson, Bernstein and Pavia, J Chem Phys, 144, 184107 (2016).

16.122 fix npt/sphere command

16.123 fix npt/sphere/omp command

16.123.1 Syntax

```
fix ID group-ID npt/sphere keyword value ...
```

- ID, group-ID are documented in *fix* command npt/sphere = style name of this fix command zero or more keyword/value pairs may be appended
- keyword = *disc*

disc value = none = treat particles as 2d discs, not spheres

- additional thermostat and barostat related keyword/value pairs from the *fix npt* command can be appended

16.123.2 Examples

```
fix 1 all npt/sphere temp 300.0 300.0 100.0 iso 0.0 0.0 1000.0
fix 2 all npt/sphere temp 300.0 300.0 100.0 x 5.0 5.0 1000.0
fix 2 all npt/sphere temp 300.0 300.0 100.0 x 5.0 5.0 1000.0 disc
fix 2 all npt/sphere temp 300.0 300.0 100.0 x 5.0 5.0 1000.0 drag 0.2
fix 2 water npt/sphere temp 300.0 300.0 100.0 aniso 0.0 0.0 1000.0 dilate partial
```

16.123.3 Description

Perform constant NPT integration to update position, velocity, and angular velocity each timestep for finite-sizex spherical particles in the group using a Nose/Hoover temperature thermostat and Nose/Hoover pressure barostat. P is pressure; T is temperature. This creates a system trajectory consistent with the isothermal-isobaric ensemble.

This fix differs from the *fix npt* command, which assumes point particles and only updates their position and velocity.

The thermostat is applied to both the translational and rotational degrees of freedom for the spherical particles, assuming a compute is used which calculates a temperature that includes the rotational degrees of freedom (see below). The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

If the *disc* keyword is used, then each particle is treated as a 2d disc (circle) instead of as a sphere. This is only possible for 2d simulations, as defined by the *dimension* keyword. The only difference between discs and spheres in this context is their moment of inertia, as used in the time integration.

Additional parameters affecting the thermostat and barostat are specified by keywords and values documented with the *fix npt* command. See, for example, discussion of the *temp*, *iso*, *aniso*, and *dilate* keywords.

The particles in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the NPT integration.

Regardless of what particles are in the fix group, a global pressure is computed for all particles. Similarly, when the size of the simulation box is changed, all particles are re-scaled to new positions, unless the keyword *dilate* is specified with a value of *partial*, in which case only the particles in the fix group are re-scaled. The latter can be useful for leaving the coordinates of particles in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp/sphere" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp all temp/sphere
compute fix-ID_press all pressure fix-ID_temp
```

See the *compute temp/sphere* and *compute pressure* commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the *compute_modify* command or print this temperature or pressure during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with *compute commands* that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the *fix_modify* command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual *compute commands* to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages*

doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover thermostat and barostat to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify* *temp* and *press* options are supported by this fix. You can use them to assign a *compute* you have defined to this fix which will be used in its thermostatting or barostatting procedure. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The *fix_modify* *energy* option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting and barostatting to the system's potential energy as part of *thermodynamic output*.

This fix computes the same global scalar and global vector of quantities as does the *fix npt* command.

This fix can ramp its target temperature and pressure over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.123.4 Restrictions

This fix requires that atoms store torque and angular velocity (omega) and a radius as defined by the *atom_style sphere* command.

All particles in the group must be finite-size spheres. They cannot be point particles.

Use of the *disc* keyword is only allowed for 2d simulations, as defined by the *dimension* keyword.

16.123.5 Related commands

fix npt, *fix nve_sphere*, *fix nvt_sphere*, *fix npt_asphere*, *fix_modify*

Default: none

16.124 fix nve command

16.125 fix nve/intel command

16.126 fix nve/kk command

16.127 fix nve/omp command

16.127.1 Syntax

```
fix ID group-ID nve
```

- ID, group-ID are documented in *fix* command
- nve = style name of this fix command

16.127.2 Examples

```
fix 1 all nve
```

16.127.3 Description

Perform constant NVE integration to update position and velocity for atoms in the group each timestep. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.127.4 Restrictions

none

16.127.5 Related commands

fix nvt, *fix npt*

Default: none

16.128 fix nve/asphere command

16.129 fix nve/asphere/intel command

16.129.1 Syntax

```
fix ID group-ID nve/asphere
```

- ID, group-ID are documented in *fix* command
- nve/asphere = style name of this fix command

16.129.2 Examples

```
fix 1 all nve/asphere
```

16.129.3 Description

Perform constant NVE integration to update position, velocity, orientation, and angular velocity for aspherical particles in the group each timestep. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble.

This fix differs from the *fix nve* command, which assumes point particles and only updates their position and velocity.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

16.129.4 Restrictions

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix requires that atoms store torque and angular momentum and a quaternion as defined by the *atom_style ellipsoid* command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or spherical as defined by their shape attribute.

16.129.5 Related commands

fix nve, *fix nve/sphere*

Default: none

16.130 fix nve/asphere/noforce command

16.130.1 Syntax

```
fix ID group-ID nve/asphere/noforce
```

- ID, group-ID are documented in *fix* command
- nve/asphere/noforce = style name of this fix command

16.130.2 Examples

fix 1 all nve/asphere/noforce

16.130.3 Description

Perform updates of position and orientation, but not velocity or angular momentum for atoms in the group each timestep. In other words, the force and torque on the atoms is ignored and their velocity and angular momentum are not updated. The atom velocities and angular momenta are used to update their positions and orientation.

This is useful as an implicit time integrator for Fast Lubrication Dynamics, since the velocity and angular momentum are updated by the *pair_style lubricuteU* command.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.130.4 Restrictions

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix requires that atoms store torque and angular momentum and a quaternion as defined by the *atom_style ellipsoid* command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or spherical as defined by their shape attribute.

16.130.5 Related commands

fix nve/noforce, *fix nve/asphere*

Default: none

16.131 fix nve/awpmd command

16.131.1 Syntax

```
fix ID group-ID nve/awpmd
```

- ID, group-ID are documented in *fix* command
- nve/awpmd = style name of this fix command

16.131.2 Examples

```
fix 1 all nve/awpmd
```

16.131.3 Description

Perform constant NVE integration to update position and velocity for nuclei and electrons in the group for the *Antisymmetrized Wave Packet Molecular Dynamics* model. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble.

The operation of this fix is exactly like that described by the *fix nve* command, except that the width and width-velocity of the electron wave functions are also updated.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.131.4 Restrictions

This fix is part of the USER-AWPMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.131.5 Related commands

fix nve

Default: none

16.132 fix nve/body command

16.132.1 Syntax

```
fix ID group-ID nve/body
```

- ID, group-ID are documented in *fix* command
- nve/body = style name of this fix command

16.132.2 Examples

```
fix 1 all nve/body
```

16.132.3 Description

Perform constant NVE integration to update position, velocity, orientation, and angular velocity for body particles in the group each timestep. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble. See the *Howto body* doc page for more details on using body particles.

This fix differs from the *fix nve* command, which assumes point particles and only updates their position and velocity.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.132.4 Restrictions

This fix is part of the BODY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix requires that atoms store torque and angular momentum and a quaternion as defined by the *atom_style body* command.

All particles in the group must be body particles. They cannot be point particles.

16.132.5 Related commands

fix nve, *fix nve/sphere*, *fix nve/asphere*

Default: none

16.133 fix nve/dot command

16.133.1 Syntax

```
fix ID group-ID nve/dot
```

- ID, group-ID are documented in *fix* command
- nve/dot = style name of this fix command

16.133.2 Examples

```
fix 1 all nve/dot
```

16.133.3 Description

Apply a rigid-body integrator as described in *(Davidchack)* to a group of atoms, but without Langevin dynamics. This command performs Molecular dynamics (MD) via a velocity-Verlet algorithm and an evolution operator that rotates the quaternion degrees of freedom, similar to the scheme outlined in *(Miller)*.

This command is the equivalent of the *fix nve/dotc/langevin* without damping and noise and can be used to determine the stability range in a NVE ensemble prior to using the Langevin-type DOTC-integrator (see also *fix nve/dotc/langevin*). The command is equivalent to the *fix nve*. The particles are always considered to have a finite size.

An example input file can be found in /examples/USER/cgdna/examples/duplex1/. Further details of the implementation and stability of the integrator are contained in *(Henrich)*. The preprint version of the article can be found here.

16.133.4 Restrictions

These pair styles can only be used if LAMMPS was built with the *USER-CGDNA* package and the MOLECULE and ASPHERE package. See the *Build package* doc page for more info.

16.133.5 Related commands

fix nve/dotc/langevin, *fix nve*

Default: none

(Davidchack) R.L Davidchack, T.E. Ouldridge, and M.V. Tretyakov. J. Chem. Phys. 142, 144114 (2015).

(Miller) T. F. Miller III, M. Eleftheriou, P. Pattnaik, A. Ndirango, G. J. Martyna, J. Chem. Phys., 116, 8649-8659 (2002).

(Henrich) O. Henrich, Y. A. Gutierrez-Fosado, T. Curk, T. E. Ouldridge, Eur. Phys. J. E 41, 57 (2018).

16.134 fix nve/dotc/langevin command

16.134.1 Syntax

```
fix ID group-ID nve/dotc/langevin Tstart Tstop damp seed keyword value
```

- ID, group-ID are documented in *fix* command
- nve/dotc/langevin = style name of this fix command
- Tstart,Tstop = desired temperature at start/end of run (temperature units)
- damp = damping parameter (time units)
- seed = random number seed to use for white noise (positive integer)
- keyword = *angmom*

  angmom value = factor
    factor = do thermostat rotational degrees of freedom via the angular momentum and apply numeric scale factor as discussed below

16.134.2 Examples

```
fix 1 all nve/dotc/langevin 1.0 1.0 0.03 457145 angmom 10
fix 1 all nve/dotc/langevin 0.1 0.1 78.9375 457145 angmom 10
```

16.134.3 Description

Apply a rigid-body Langevin-type integrator of the kind "Langevin C" as described in *(Davidchack)* to a group of atoms, which models an interaction with an implicit background solvent. This command performs Brownian dynamics (BD) via a technique that splits the integration into a deterministic Hamiltonian part and the Ornstein-Uhlenbeck process for noise and damping. The quaternion degrees of freedom are updated though an evolution operator which performs a rotation in quaternion space, preserves the quaternion norm and is akin to *(Miller)*.

In terms of syntax this command has been closely modelled on the *fix langevin* and its *angmom* option. But it combines the *fix nve* and the *fix langevin* in one single command. The main feature is improved stability over the standard integrator, permitting slightly larger timestep sizes.

Note: Unlike the *fix langevin* this command performs also time integration of the translational and quaternion degrees of freedom.

The total force on each atom will have the form:

$$
\begin{aligned}
F =& F_c + F_f + F_r \\
F_f =& -\frac{m}{\mathrm{damp}} v \\
F_r \propto& \sqrt{\frac{k_B T m}{dt\ \mathrm{damp}}}
\end{aligned}
$$

F_c is the conservative force computed via the usual inter-particle interactions (*pair_style*, *bond_style*, etc). The F_f and F_r terms are implicitly taken into account by this fix on a per-particle basis.

F_f is a frictional drag or viscous damping term proportional to the particle's velocity. The proportionality constant for each atom is computed as $\frac{m}{\mathrm{damp}}$, where *m* is the mass of the particle and damp is the damping factor specified by the user.

F_r is a force due to solvent atoms at a temperature *T* randomly bumping into the particle. As derived from the fluctuation/dissipation theorem, its magnitude as shown above is proportional to $\sqrt{\frac{k_B T m}{dt\ \mathrm{damp}}}$, where k_B is the Boltzmann constant, *T* is the desired temperature, *m* is the mass of the particle, *dt* is the timestep size, and damp is the damping factor. Random numbers are used to randomize the direction and magnitude of this force as described in *(Dunweg)*, where a uniform random number is used (instead of a Gaussian random number) for speed.

Tstart and *Tstop* have to be constant values, i.e. they cannot be variables. If used together with the oxDNA force field for coarse-grained simulation of DNA please note that T = 0.1 in oxDNA units corresponds to T = 300 K.

The *damp* parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 0.03 means to relax the temperature in a timespan of (roughly) 0.03 time units tau (see the *units* command). The damp factor can be thought of as inversely related to the viscosity of the solvent, i.e. a small relaxation time implies a high-viscosity solvent and vice versa. See the discussion about gamma and viscosity in the documentation for the *fix viscous* command for more details. Note that the value 78.9375 in the second example above corresponds to a diffusion constant, which is about an order of magnitude larger than realistic ones. This has been used to sample configurations faster in Brownian dynamics simulations.

The random # *seed* must be a positive integer. A Marsaglia random number generator is used. Each processor uses the input seed to generate its own unique seed and its own stream of random numbers. Thus the dynamics of the system will not be identical on two runs on different numbers of processors.

The keyword/value option has to be used in the following way:

This fix has to be used together with the *angmom* keyword. The particles are always considered to have a finite size. The keyword *angmom* enables thermostatting of the rotational degrees of freedom in addition to the usual translational degrees of freedom.

The scale factor after the *angmom* keyword gives the ratio of the rotational to the translational friction coefficient.

An example input file can be found in examples/USER/cgdna/examples/duplex2/. Further details of the implementation and stability of the integrators are contained in *(Henrich)*. The preprint version of the article can be found here.

16.134.4 Restrictions

These pair styles can only be used if LAMMPS was built with the *USER-CGDNA* package and the MOLECULE and ASPHERE package. See the *Build package* doc page for more info.

16.134.5 Related commands

fix nve, *fix langevin*, *fix nve/dot*, *bond_style oxdna/fene*, *bond_style oxdna2/fene*, *pair_style oxdna/excv*, *pair_style oxdna2/excv*

Default: none

(Davidchack) R.L Davidchack, T.E. Ouldridge, M.V. Tretyakov. J. Chem. Phys. 142, 144114 (2015).

(Miller) T. F. Miller III, M. Eleftheriou, P. Pattnaik, A. Ndirango, G. J. Martyna, J. Chem. Phys., 116, 8649-8659 (2002).

(Dunweg) B. Dunweg, W. Paul, Int. J. Mod. Phys. C, 2, 817-27 (1991).

(Henrich) O. Henrich, Y. A. Gutierrez-Fosado, T. Curk, T. E. Ouldridge, Eur. Phys. J. E 41, 57 (2018).

16.135 fix nve/eff command

16.135.1 Syntax

```
fix ID group-ID nve/eff
```

- ID, group-ID are documented in *fix* command
- nve/eff = style name of this fix command

16.135.2 Examples

```
fix 1 all nve/eff
```

16.135.3 Description

Perform constant NVE integration to update position and velocity for nuclei and electrons in the group for the *electron force field* model. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble.

The operation of this fix is exactly like that described by the *fix nve* command, except that the radius and radial velocity of electrons are also updated.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.135.4 Restrictions

This fix is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.135.5 Related commands

fix nve, *fix nvt/eff*, *fix npt/eff*

Default: none

16.136 fix nve/limit command

16.136.1 Syntax

```
fix ID group-ID nve/limit xmax
```

- ID, group-ID are documented in *fix* command
- nve = style name of this fix command
- xmax = maximum distance an atom can move in one timestep (distance units)

16.136.2 Examples

```
fix 1 all nve/limit 0.1
```

16.136.3 Description

Perform constant NVE updates of position and velocity for atoms in the group each timestep. A limit is imposed on the maximum distance an atom can move in one timestep. This is useful when starting a simulation with a configuration containing highly overlapped atoms. Normally this would generate huge forces which would blow atoms out of the simulation box, causing LAMMPS to stop with an error.

Using this fix can overcome that problem. Forces on atoms must still be computable (which typically means 2 atoms must have a separation distance > 0.0). But large velocities generated by large forces are reset to a value that corresponds to a displacement of length *xmax* in a single timestep. *Xmax* is specified in distance units; see the *units* command for details. The value of *xmax* should be consistent with the neighbor skin distance and the frequency of neighbor list re-building, so that pairwise interactions are not missed on successive timesteps as atoms move. See the *neighbor* and *neigh_modify* commands for details.

Note that if a velocity reset occurs the integrator will not conserve energy. On steps where no velocity resets occur, this integrator is exactly like the *fix nve* command. Since forces are unaltered, pressures computed by thermodynamic output will still be very large for overlapped configurations.

Note: You should not use *fix shake* in conjunction with this fix. That is because fix shake applies constraint forces based on the predicted positions of atoms after the next timestep. It has no way of knowing the timestep may change due to this fix, which will cause the constraint forces to be invalid. A better strategy is to turn off fix shake when performing initial dynamics that need this fix, then turn fix shake on when doing normal dynamics with a fixed-size timestep.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the count of how many updates of atom's velocity/position were limited by the maximum distance criterion. This should be roughly the number of atoms so affected, except that updates occur at both the beginning and end of a timestep in a velocity Verlet timestepping algorithm. This is a cumulative quantity for the current run, but is re-initialized to zero each time a run is performed. The scalar value calculated by this fix is "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.136.4 Restrictions

none

16.136.5 Related commands

fix nve, *fix nve/noforce*, *pair_style soft*

Default: none

16.137 fix nve/line command

16.137.1 Syntax

```
fix ID group-ID nve/line
```

- ID, group-ID are documented in *fix* command
- nve/line = style name of this fix command

16.137.2 Examples

```
fix 1 all nve/line
```

16.137.3 Description

Perform constant NVE integration to update position, velocity, orientation, and angular velocity for line segment particles in the group each timestep. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble. See *Howto spherical* doc page for an overview of using line segment particles.

This fix differs from the *fix nve* command, which assumes point particles and only updates their position and velocity.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.137.4 Restrictions

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix requires that particles be line segments as defined by the *atom_style line* command.

16.137.5 Related commands

fix nve, *fix nve/asphere*

Default: none

16.138 fix nve/manifold/rattle command

16.138.1 Syntax

```
fix ID group-ID nve/manifold/rattle tol maxit manifold manifold-args keyword value ...
```

- ID, group-ID are documented in *fix* command
- nve/manifold/rattle = style name of this fix command
- tol = tolerance to which Newton iteration must converge
- maxit = maximum number of iterations to perform
- manifold = name of the manifold
- manifold-args = parameters for the manifold
- one or more keyword/value pairs may be appended

```
keyword = every
  every values = N
    N = print info about iteration every N steps. N = 0 means no output
```

16.138.2 Examples

```
fix 1 all nve/manifold/rattle 1e-4 10 sphere 5.0
fix step all nve/manifold/rattle 1e-8 100 ellipsoid 2.5 2.5 5.0 every 25
```

16.138.3 Description

Perform constant NVE integration to update position and velocity for atoms constrained to a curved surface (manifold) in the group each timestep. The constraint is handled by RATTLE *(Andersen)* written out for the special case of single-particle constraints as explained in *(Paquay)*. V is volume; E is energy. This way, the dynamics of particles constrained to curved surfaces can be studied. If combined with *fix langevin*, this generates Brownian motion of particles constrained to a curved surface. For a list of currently supported manifolds and their parameters, see the *Howto manifold* doc page.

Note that the particles must initially be close to the manifold in question. If not, RATTLE will not be able to iterate until the constraint is satisfied, and an error is generated. For simple manifolds this can be achieved with *region* and *create_atoms* commands, but for more complex surfaces it might be more useful to write a script.

The manifold args may be equal-style variables, like so:

```
variable R equal "ramp(5.0,3.0)"
fix shrink_sphere all nve/manifold/rattle 1e-4 10 sphere v_R
```

In this case, the manifold parameter will change in time according to the variable. This is not a problem for the time integrator as long as the change of the manifold is slow with respect to the dynamics of the particles. Note that if the manifold has to exert work on the particles because of these changes, the total energy might not be conserved.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.138.4 Restrictions

This fix is part of the USER-MANIFOLD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.138.5 Related commands

fix nvt/manifold/rattle, *fix manifoldforce*

Default: every = 0, tchain = 3

(Andersen) Andersen, J. Comp. Phys. 52, 24, (1983).

(Paquay) Paquay and Kusters, Biophys. J., 110, 6, (2016). preprint available at arXiv:1411.3019.

16.139 fix nve/noforce command

16.139.1 Syntax

```
fix ID group-ID nve
```

- ID, group-ID are documented in *fix* command
- nve/noforce = style name of this fix command

16.139.2 Examples

```
fix 3 wall nve/noforce
```

16.139.3 Description

Perform updates of position, but not velocity for atoms in the group each timestep. In other words, the force on the atoms is ignored and their velocity is not updated. The atom velocities are used to update their positions.

This can be useful for wall atoms, when you set their velocities, and want the wall to move (or stay stationary) in a prescribed fashion.

This can also be accomplished via the *fix setforce* command, but with fix nve/noforce, the forces on the wall atoms are unchanged, and can thus be printed by the *dump* command or queried with an equal-style *variable* that uses the fcm() group function to compute the total force on the group of atoms.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.139.4 Restrictions

none

16.139.5 Related commands

fix nve

Default: none

16.140 fix nve/sphere command

16.141 fix nve/sphere/omp command

16.142 fix nve/sphere/kk command

16.142.1 Syntax

```
fix ID group-ID nve/sphere
```

- ID, group-ID are documented in *fix* command
- nve/sphere = style name of this fix command
- zero or more keyword/value pairs may be appended
- keyword = *update* or *disc*

```
update value = dipole or dipole/dlm
  dipole = update orientation of dipole moment during integration
  dipole/dlm = use DLM integrator to update dipole orientation
disc value = none = treat particles as 2d discs, not spheres
```

16.142.2 Examples

```
fix 1 all nve/sphere
fix 1 all nve/sphere update dipole
fix 1 all nve/sphere disc
fix 1 all nve/sphere update dipole/dlm
```

16.142.3 Description

Perform constant NVE integration to update position, velocity, and angular velocity for finite-size spherical particles in the group each timestep. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble.

This fix differs from the *fix nve* command, which assumes point particles and only updates their position and velocity.

If the *update* keyword is used with the *dipole* value, then the orientation of the dipole moment of each particle is also updated during the time integration. This option should be used for models where a dipole moment is assigned to finite-size particles, e.g. spheroids via use of the *atom_style hybrid sphere dipole* command.

The default dipole orientation integrator can be changed to the Dullweber-Leimkuhler-McLachlan integration scheme *(Dullweber)* when using *update* with the value *dipole/dlm*. This integrator is symplectic and time-reversible, giving better energy conservation and allows slightly longer timesteps at only a small additional computational cost.

If the *disc* keyword is used, then each particle is treated as a 2d disc (circle) instead of as a sphere. This is only possible for 2d simulations, as defined by the *dimension* keyword. The only difference between discs and spheres in this context is their moment of inertia, as used in the time integration.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.142.4 Restrictions

This fix requires that atoms store torque and angular velocity (omega) and a radius as defined by the *atom_style sphere* command. If the *dipole* keyword is used, then they must also store a dipole moment as defined by the *atom_style dipole* command.

All particles in the group must be finite-size spheres. They cannot be point particles.

Use of the *disc* keyword is only allowed for 2d simulations, as defined by the *dimension* keyword.

16.142.5 Related commands

fix nve, *fix nve/asphere*

Default: none

(Dullweber) Dullweber, Leimkuhler and McLachlan, J Chem Phys, 107, 5840 (1997).

16.143 fix nve/spin command

16.143.1 Syntax

```
fix ID group-ID nve/spin keyword values
```

- ID, group-ID are documented in *fix* command
- nve/spin = style name of this fix command
- keyword = *lattice*

```
lattice value = moving or frozen
  moving = integrate both spin and atomic degress of freedom
  frozen = integrate spins on a fixed lattice
```

16.143.2 Examples

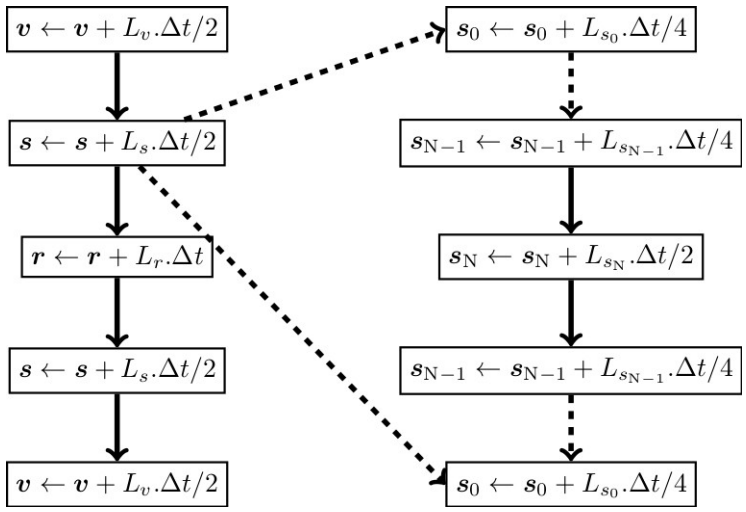
```
fix 3 all nve/spin lattice moving
fix 1 all nve/spin lattice frozen
```

16.143.3 Description

Perform a symplectic integration for the spin or spin-lattice system.

The *lattice* keyword defines if the spins are integrated on a lattice of fixed atoms (lattice = frozen), or if atoms are moving (lattice = moving). The first case corresponds to a spin dynamics calculation, and the second to a spin-lattice calculation. By default a spin-lattice integration is performed (lattice = moving).

The *nve/spin* fix applies a Suzuki-Trotter decomposition to the equations of motion of the spin lattice system, following the scheme:



according to the implementation reported in *(Omelyan)*.

A sectoring method enables this scheme for parallel calculations. The implementation of this sectoring algorithm is reported in *(Tranchida)*.

16.143.4 Restrictions

This fix style can only be used if LAMMPS was built with the SPIN package. See the *Build package* doc page for more info.

To use the spin algorithm, it is necessary to define a map with the atom_modify command. Typically, by adding the command:

```
atom_modify map array
```

before you create the simulation box. Note that the keyword "hash" instead of "array" is also valid.

16.143.5 Related commands

atom_style spin, *fix nve*

16.143.6 Default

The option default is lattice = moving.

(Omelyan) Omelyan, Mryglod, and Folk. Phys. Rev. Lett. 86(5), 898. (2001).

(Tranchida) Tranchida, Plimpton, Thibaudeau and Thompson, Journal of Computational Physics, 372, 406-425, (2018).

16.144 fix nve/tri command

16.144.1 Syntax

```
fix ID group-ID nve/tri
```

- ID, group-ID are documented in *fix* command
- nve/tri = style name of this fix command

16.144.2 Examples

```
fix 1 all nve/tri
```

16.144.3 Description

Perform constant NVE integration to update position, velocity, orientation, and angular momentum for triangular particles in the group each timestep. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble. See the *Howto spherical* doc page for an overview of using triangular particles.

This fix differs from the *fix nve* command, which assumes point particles and only updates their position and velocity.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.144.4 Restrictions

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix requires that particles be triangles as defined by the *atom_style tri* command.

16.144.5 Related commands

fix nve, *fix nve/asphere*

Default: none

16.145 fix nvk command

16.145.1 Syntax

```
fix ID group-ID nvk
```

- ID, group-ID are documented in *fix* command
- nvk = style name of this fix command

16.145.2 Examples

```
fix 1 all nvk
```

16.145.3 Description

Perform constant kinetic energy integration using the Gaussian thermostat to update position and velocity for atoms in the group each timestep. V is volume; K is kinetic energy. This creates a system trajectory consistent with the isokinetic ensemble.

The equations of motion used are those of Minary et al in *(Minary)*, a variant of those initially given by Zhang in *(Zhang)*.

The kinetic energy will be held constant at its value given when fix nvk is initiated. If a different kinetic energy is desired, the *velocity* command should be used to change the kinetic energy prior to this fix.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.145.4 Restrictions

The Gaussian thermostat only works when it is applied to all atoms in the simulation box. Therefore, the group must be set to all.

This fix has not yet been implemented to work with the RESPA integrator.

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Related commands: none

Default: none

(Minary) Minary, Martyna, and Tuckerman, J Chem Phys, 18, 2510 (2003).

(Zhang) Zhang, J Chem Phys, 106, 6102 (1997).

16.146 fix nvt/asphere command

16.147 fix nvt/asphere/omp command

16.147.1 Syntax

```
fix ID group-ID nvt/asphere keyword value ...
```

- ID, group-ID are documented in *fix* command
- nvt/asphere = style name of this fix command

- additional thermostat related keyword/value pairs from the *fix nvt* command can be appended

16.147.2 Examples

```
fix 1 all nvt/asphere temp 300.0 300.0 100.0
fix 1 all nvt/asphere temp 300.0 300.0 100.0 drag 0.2
```

16.147.3 Description

Perform constant NVT integration to update position, velocity, orientation, and angular velocity each timestep for aspherical or ellipsoidal particles in the group using a Nose/Hoover temperature thermostat. V is volume; T is temperature. This creates a system trajectory consistent with the canonical ensemble.

This fix differs from the *fix nvt* command, which assumes point particles and only updates their position and velocity.

The thermostat is applied to both the translational and rotational degrees of freedom for the aspherical particles, assuming a compute is used which calculates a temperature that includes the rotational degrees of freedom (see below). The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

Additional parameters affecting the thermostat are specified by keywords and values documented with the *fix nvt* command. See, for example, discussion of the *temp* and *drag* keywords.

This fix computes a temperature each timestep. To do this, the fix creates its own compute of style "temp/asphere", as if this command had been issued:

```
compute fix-ID_temp group-ID temp/asphere
```

See the *compute temp/asphere* command for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp*. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the *compute_modify* command or print this temperature during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with *compute commands* that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the *fix_modify* command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual *compute commands* to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover thermostat to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify* *temp* option is supported by this fix. You can use it to assign a *compute* you have defined to this fix which will be used in its thermostatting procedure.

The *fix_modify* *energy* option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting to the system's potential energy as part of *thermodynamic output*.

This fix computes the same global scalar and global vector of quantities as does the *fix nvt* command.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.147.4 Restrictions

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix requires that atoms store torque and angular momentum and a quaternion as defined by the *atom_style ellipsoid* command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or spherical as defined by their shape attribute.

16.147.5 Related commands

fix nvt, *fix nve_asphere*, *fix npt_asphere*, *fix_modify*

Default: none

16.148 fix nvt/body command

16.148.1 Syntax

```
fix ID group-ID nvt/body keyword value ...
```

- ID, group-ID are documented in *fix* command
- nvt/body = style name of this fix command
- additional thermostat related keyword/value pairs from the *fix nvt* command can be appended

16.148.2 Examples

```
fix 1 all nvt/body temp 300.0 300.0 100.0
fix 1 all nvt/body temp 300.0 300.0 100.0 drag 0.2
```

16.148.3 Description

Perform constant NVT integration to update position, velocity, orientation, and angular velocity each timestep for body particles in the group using a Nose/Hoover temperature thermostat. V is volume; T is temperature. This creates a system trajectory consistent with the canonical ensemble.

This fix differs from the *fix nvt* command, which assumes point particles and only updates their position and velocity.

The thermostat is applied to both the translational and rotational degrees of freedom for the body particles, assuming a compute is used which calculates a temperature that includes the rotational degrees of freedom (see below). The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

Additional parameters affecting the thermostat are specified by keywords and values documented with the *fix nvt* command. See, for example, discussion of the *temp* and *drag* keywords.

This fix computes a temperature each timestep. To do this, the fix creates its own compute of style "temp/body", as if this command had been issued:

```
compute fix-ID_temp group-ID temp/body
```

See the *compute temp/body* command for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp*. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the *compute_modify* command or print this temperature during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with *compute commands* that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the *fix_modify* command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual *compute commands* to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover thermostat to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify* *temp* option is supported by this fix. You can use it to assign a *compute* you have defined to this fix which will be used in its thermostatting procedure.

The *fix_modify* *energy* option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting to the system's potential energy as part of *thermodynamic output*.

This fix computes the same global scalar and global vector of quantities as does the *fix nvt* command.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.148.4 Restrictions

This fix is part of the BODY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix requires that atoms store torque and angular momentum and a quaternion as defined by the *atom_style body* command.

16.148.5 Related commands

fix nvt, *fix nve_body*, *fix npt_body*, *fix_modify*

Default: none

16.149 fix nvt/manifold/rattle command

16.149.1 Syntax

```
fix ID group-ID nvt/manifold/rattle tol maxit manifold manifold-args keyword value ...
```

- ID, group-ID are documented in *fix* command
- nvt/manifold/rattle = style name of this fix command
- tol = tolerance to which Newton iteration must converge
- maxit = maximum number of iterations to perform
- manifold = name of the manifold
- manifold-args = parameters for the manifold
- one or more keyword/value pairs may be appended

```
keyword = temp or tchain or every
  temp values = Tstart Tstop Tdamp
    Tstart, Tstop = external temperature at start/end of run
    Tdamp = temperature damping parameter (time units)
  tchain value = N
```

```
    N = length of thermostat chain (1 = single thermostat)
  every value = N
    N = print info about iteration every N steps. N = 0 means no output
```

16.149.2 Examples

fix 1 all nvt/manifold/rattle 1e-4 10 cylinder 3.0 temp 1.0 1.0 10.0

16.149.3 Description

This fix combines the RATTLE-based *(Andersen)* time integrator of *fix nve/manifold/rattle (Paquay)* with a Nose-Hoover-chain thermostat to sample the canonical ensemble of particles constrained to a curved surface (manifold). This sampling does suffer from discretization bias of O(dt). For a list of currently supported manifolds and their parameters, see the *Howto manifold* doc page.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.149.4 Restrictions

This fix is part of the USER-MANIFOLD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.149.5 Related commands

fix nve/manifold/rattle, *fix manifoldforce* **Default:** every = 0

(Andersen) Andersen, J. Comp. Phys. 52, 24, (1983).

(Paquay) Paquay and Kusters, Biophys. J., 110, 6, (2016). preprint available at arXiv:1411.3019.

16.150 fix nvt/sllod command

16.151 fix nvt/sllod/intel command

16.152 fix nvt/sllod/omp command

16.152.1 Syntax

```
fix ID group-ID nvt/sllod keyword value ...
```

- ID, group-ID are documented in *fix* command
- nvt/sllod = style name of this fix command
- additional thermostat related keyword/value pairs from the *fix nvt* command can be appended

16.152.2 Examples

```
fix 1 all nvt/sllod temp 300.0 300.0 100.0
fix 1 all nvt/sllod temp 300.0 300.0 100.0 drag 0.2
```

16.152.3 Description

Perform constant NVT integration to update positions and velocities each timestep for atoms in the group using a Nose/Hoover temperature thermostat. V is volume; T is temperature. This creates a system trajectory consistent with the canonical ensemble.

This thermostat is used for a simulation box that is changing size and/or shape, for example in a non-equilibrium MD (NEMD) simulation. The size/shape change is induced by use of the *fix deform* command, so each point in the simulation box can be thought of as having a "streaming" velocity. This position-dependent streaming velocity is subtracted from each atom's actual velocity to yield a thermal velocity which is used for temperature computation and thermostatting. For example, if the box is being sheared in x, relative to y, then points at the bottom of the box (low y) have a small x velocity, while points at the top of the box (hi y) have a large x velocity. These velocities do not contribute to the thermal "temperature" of the atom.

Note: *Fix deform* has an option for remapping either atom coordinates or velocities to the changing simulation box. To use fix nvt/sllod, fix deform should NOT remap atom positions, because fix nvt/sllod adjusts the atom positions and velocities to create a velocity profile that matches the changing box size/shape. Fix deform SHOULD remap atom velocities when atoms cross periodic boundaries since that is consistent with maintaining the velocity profile created by fix nvt/sllod. LAMMPS will give an error if this setting is not consistent.

The SLLOD equations of motion, originally proposed by Hoover and Ladd (see *(Evans and Morriss)*), were proven to be equivalent to Newton's equations of motion for shear flow by *(Evans and Morriss)*. They were later shown to generate the desired velocity gradient and the correct production of work by stresses for all forms of homogeneous flow by *(Daivis and Todd)*. As implemented in LAMMPS, they are coupled to a Nose/Hoover chain thermostat in a velocity Verlet formulation, closely following the implementation used for the *fix nvt* command.

Note: A recent (2017) book by *(Daivis and Todd)* discusses use of the SLLOD method and non-equilibrium MD (NEMD) thermostatting generally, for both simple and complex fluids, e.g. molecular systems. The latter can be tricky to do correctly.

Additional parameters affecting the thermostat are specified by keywords and values documented with the *fix nvt* command. See, for example, discussion of the *temp* and *drag* keywords.

This fix computes a temperature each timestep. To do this, the fix creates its own compute of style "temp/deform", as if this command had been issued:

```
compute fix-ID_temp group-ID temp/deform
```

See the *compute temp/deform* command for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp*. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the *compute_modify* command or print this temperature during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with *compute commands* that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the *fix_modify* command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual *compute commands* to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover thermostat to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify temp* option is supported by this fix. You can use it to assign a *compute* you have defined to this fix which will be used in its thermostatting procedure.

The *fix_modify energy* option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting to the system's potential energy as part of *thermodynamic output*.

This fix computes the same global scalar and global vector of quantities as does the *fix nvt* command.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.152.4 Restrictions

This fix works best without Nose-Hoover chain thermostats, i.e. using tchain = 1. Setting tchain to larger values can result in poor equilibration.

16.152.5 Related commands

fix nve, *fix nvt*, *fix temp/rescale*, *fix langevin*, *fix_modify*, *compute temp/deform*

16.152.6 Default

Same as *fix nvt*, except tchain = 1.

(Evans and Morriss) Evans and Morriss, Phys Rev A, 30, 1528 (1984).

(Daivis and Todd) Daivis and Todd, J Chem Phys, 124, 194103 (2006).

(Daivis and Todd) Daivis and Todd, Nonequilibrium Molecular Dynamics (book), Cambridge University Press, https://doi.org/10.1017/9781139017848, (2017).

16.153 fix nvt/sllod/eff command

16.153.1 Syntax

```
fix ID group-ID nvt/sllod/eff keyword value ...
```

- ID, group-ID are documented in *fix* command
- nvt/sllod/eff = style name of this fix command
- additional thermostat related keyword/value pairs from the *fix nvt/eff* command can be appended

16.153.2 Examples

```
fix 1 all nvt/sllod/eff temp 300.0 300.0 0.1
fix 1 all nvt/sllod/eff temp 300.0 300.0 0.1 drag 0.2
```

16.153.3 Description

Perform constant NVT integration to update positions and velocities each timestep for nuclei and electrons in the group for the *electron force field* model, using a Nose/Hoover temperature thermostat. V is volume; T is temperature. This creates a system trajectory consistent with the canonical ensemble.

The operation of this fix is exactly like that described by the *fix nvt/sllod* command, except that the radius and radial velocity of electrons are also updated and thermostatted. Likewise the temperature calculated by the fix, using the compute it creates (as discussed in the *fix nvt, npt, and nph* doc page), is performed with a *compute temp/deform/eff* command that includes the eFF contribution to the temperature from the electron radial velocity.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover thermostat to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify* *temp* option is supported by this fix. You can use it to assign a *compute* you have defined to this fix which will be used in its thermostatting procedure.

The *fix_modify* *energy* option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting to the system's potential energy as part of *thermodynamic output*.

This fix computes the same global scalar and global vector of quantities as does the *fix nvt/eff* command.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.153.4 Restrictions

This fix is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix works best without Nose-Hoover chain thermostats, i.e. using tchain = 1. Setting tchain to larger values can result in poor equilibration.

16.153.5 Related commands

fix nve/eff, *fix nvt/eff*, *fix langevin/eff*, *fix nvt/sllod*, *fix_modify*, *compute temp/deform/eff*

16.153.6 Default

Same as *fix nvt/eff*, except tchain = 1.

(Tuckerman) Tuckerman, Mundy, Balasubramanian, Klein, J Chem Phys, 106, 5615 (1997).

16.154 fix nvt/sphere command

16.155 fix nvt/sphere/omp command

16.155.1 Syntax

```
fix ID group-ID nvt/sphere keyword value ...
```

- ID, group-ID are documented in *fix* command
- nvt/sphere = style name of this fix command
- zero or more keyword/value pairs may be appended
- keyword = *disc*

  disc value = none = treat particles as 2d discs, not spheres

- additional thermostat related keyword/value pairs from the *fix nvt* command can be appended

16.155.2 Examples

```
fix 1 all nvt/sphere temp 300.0 300.0 100.0
fix 1 all nvt/sphere temp 300.0 300.0 100.0 disc
fix 1 all nvt/sphere temp 300.0 300.0 100.0 drag 0.2
```

16.155.3 Description

Perform constant NVT integration to update position, velocity, and angular velocity each timestep for finite-size spherical particles in the group using a Nose/Hoover temperature thermostat. V is volume; T is temperature. This creates a system trajectory consistent with the canonical ensemble.

This fix differs from the *fix nvt* command, which assumes point particles and only updates their position and velocity.

The thermostat is applied to both the translational and rotational degrees of freedom for the spherical particles, assuming a compute is used which calculates a temperature that includes the rotational degrees of freedom (see below). The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

If the *disc* keyword is used, then each particle is treated as a 2d disc (circle) instead of as a sphere. This is only possible for 2d simulations, as defined by the *dimension* keyword. The only difference between discs and spheres in this context is their moment of inertia, as used in the time integration.

Additional parameters affecting the thermostat are specified by keywords and values documented with the *fix nvt* command. See, for example, discussion of the *temp* and *drag* keywords.

This fix computes a temperature each timestep. To do this, the fix creates its own compute of style "temp/sphere", as if this command had been issued:

```
compute fix-ID_temp group-ID temp/sphere
```

See the *compute temp/sphere* command for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp*. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the *compute_modify* command or print this temperature during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with *compute commands* that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the *fix_modify* command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual *compute commands* to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover thermostat to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify* *temp* option is supported by this fix. You can use it to assign a *compute* you have defined to this fix which will be used in its thermostatting procedure.

The *fix_modify* *energy* option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting to the system's potential energy as part of *thermodynamic output*.

This fix computes the same global scalar and global vector of quantities as does the *fix nvt* command.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.155.4 Restrictions

This fix requires that atoms store torque and angular velocity (omega) and a radius as defined by the *atom_style sphere* command.

All particles in the group must be finite-size spheres. They cannot be point particles.

Use of the *disc* keyword is only allowed for 2d simulations, as defined by the *dimension* keyword.

16.155.5 Related commands

fix nvt, *fix nve_sphere*, *fix nvt_asphere*, *fix npt_sphere*, *fix_modify*

Default: none

16.156 fix oneway command

16.156.1 Syntax

```
fix ID group-ID oneway N region-ID direction
```

- ID, group-ID are documented in *fix* command
- oneway = style name of this fix command
- N = apply this fix every this many timesteps
- region-ID = ID of region where fix is active
- direction = *x* or *-x* or *y* or *-y* or *z* or *-z* = coordinate and direction of the oneway constraint

16.156.2 Examples

```
fix ions oneway 10 semi -x
fix all oneway 1 left -z
fix all oneway 1 right z
```

16.156.3 Description

Enforce that particles in the group and in a given region can only move in one direction. This is done by reversing a particle's velocity component, if it has the wrong sign in the specified dimension. The effect is that the particle moves in one direction only.

This can be used, for example, as a simple model of a semi-permeable membrane, or as an implementation of Maxwell's demon.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.156.4 Restrictions

none

16.156.5 Related commands

fix wall/reflect command

Default: none

16.157 fix orient/fcc command

16.158 fix orient/bcc command

```
fix ID group-ID orient/fcc nstats dir alat dE cutlo cuthi file0 file1
fix ID group-ID orient/bcc nstats dir alat dE cutlo cuthi file0 file1
```

- ID, group-ID are documented in *fix* command
- nstats = print stats every this many steps, 0 = never
- dir = 0/1 for which crystal is used as reference
- alat = fcc/bcc cubic lattice constant (distance units)
- dE = energy added to each atom (energy units)
- cutlo,cuthi = values between 0.0 and 1.0, cutlo < cuthi
- file0,file1 = files that specify orientation of each grain

16.158.1 Examples

```
fix gb all orient/fcc 0 1 4.032008 0.001 0.25 0.75 xi.vec chi.vec
fix gb all orient/bcc 0 1 2.882 0.001 0.25 0.75 ngb.left ngb.right
```

16.158.2 Description

The fix applies an orientation-dependent force to atoms near a planar grain boundary which can be used to induce grain boundary migration (in the direction perpendicular to the grain boundary plane). The motivation and explanation of this force and its application are described in *(Janssens)*. The adaptation to bcc crystals is described in *(Wicaksono1)*. The computed force is only applied to atoms in the fix group.

The basic idea is that atoms in one grain (on one side of the boundary) have a potential energy dE added to them. Atoms in the other grain have 0.0 potential energy added. Atoms near the boundary (whose neighbor environment is intermediate between the two grain orientations) have an energy between 0.0 and dE added. This creates an effective driving force to reduce the potential energy of atoms near the boundary by pushing them towards one of the grain orientations. For dir = 1 and dE > 0, the boundary will thus move so that the grain described by file0 grows and the grain described by file1 shrinks. Thus this fix is designed for simulations of two-grain systems, either with one grain boundary and free surfaces parallel to the boundary, or a system with periodic boundary conditions and two equal and opposite grain boundaries. In either case, the entire system can displace during the simulation, and such motion should be accounted for in measuring the grain boundary velocity.

The potential energy added to atom I is given by these formulas

$$\xi_i = \sum_{j=1}^{12} \left|\mathbf{r}_j - \mathbf{r}_j^{\mathrm{I}}\right| \qquad (1)$$

$$\xi_{\mathrm{IJ}} = \sum_{j=1}^{12} \left|\mathbf{r}_j^{\mathrm{J}} - \mathbf{r}_j^{\mathrm{I}}\right| \qquad (2)$$

$$\xi_{\mathrm{low}} = \mathrm{cutlo}\,\xi_{\mathrm{IJ}} \qquad (3)$$

$$\xi_{\mathrm{high}} = \mathrm{cuthi}\,\xi_{\mathrm{IJ}} \qquad (4)$$

$$\omega_i = \frac{\pi}{2}\frac{\xi_i - \xi_{\mathrm{low}}}{\xi_{\mathrm{high}} - \xi_{\mathrm{low}}} \qquad (5)$$

$$\begin{aligned} u_i &= 0 && \text{for} \quad \xi_i < \xi_{\mathrm{low}} \\ &= \mathrm{dE}\,\frac{1-\cos(2\omega_i)}{2} && \text{for} \quad \xi_{\mathrm{low}} < \xi_i < \xi_{\mathrm{high}} \qquad (6) \\ &= \mathrm{dE} && \text{for} \quad \xi_{\mathrm{high}} < \xi_i \end{aligned}$$

which are fully explained in *(Janssens)*. For fcc crystals this order parameter Xi for atom I in equation (1) is a sum over the 12 nearest neighbors of atom I. For bcc crystals it is the corresponding sum of the 8 nearest neighbors. Rj is the vector from atom I to its neighbor J, and RIj is a vector in the reference (perfect) crystal. That is, if dir = 0/1, then RIj is a vector to an atom coord from file 0/1. Equation (2) gives the expected value of the order parameter XiIJ in the other grain. Hi and lo cutoffs are defined in equations (3) and (4), using the input parameters *cutlo* and *cuthi* as thresholds to avoid adding grain boundary energy when the deviation in the order parameter from 0 or 1 is small (e.g. due to thermal fluctuations in a perfect crystal). The added potential energy Ui for atom I is given in equation (6) where it is interpolated between 0 and dE using the two threshold Xi values and the Wi value of equation (5).

The derivative of this energy expression gives the force on each atom which thus depends on the orientation of its neighbors relative to the 2 grain orientations. Only atoms near the grain boundary feel a net force which tends to drive them to one of the two grain orientations.

In equation (1), the reference vector used for each neighbor is the reference vector closest to the actual neighbor position. This means it is possible two different neighbors will use the same reference vector. In such cases, the atom in question is far from a perfect orientation and will likely receive the full dE addition, so the effect of duplicate reference vector usage is small.

The *dir* parameter determines which grain wants to grow at the expense of the other. A value of 0 means the first grain will shrink; a value of 1 means it will grow. This assumes that *dE* is positive. The reverse will be true if *dE* is negative.

The *alat* parameter is the cubic lattice constant for the fcc or bcc material and is only used to compute a cutoff distance of 1.57 * alat / sqrt(2) for finding the 12 or 8 nearest neighbors of each atom (which should be valid for an fcc or bcc crystal). A longer/shorter cutoff can be imposed by adjusting *alat*. If a particular atom has less than 12 or 8 neighbors within the cutoff, the order parameter of equation (1) is effectively multiplied by 12 or 8 divided by the actual number of neighbors within the cutoff.

The *dE* parameter is the maximum amount of additional energy added to each atom in the grain which wants to shrink.

The *cutlo* and *cuthi* parameters are used to reduce the force added to bulk atoms in each grain far away from the boundary. An atom in the bulk surrounded by neighbors at the ideal grain orientation would compute an order parameter of 0 or 1 and have no force added. However, thermal vibrations in the solid will cause the order parameters to be greater than 0 or less than 1. The cutoff parameters mask this effect, allowing forces to only be added to atoms with order-parameters between the cutoff values.

File0 and *file1* are filenames for the two grains which each contain 6 vectors (6 lines with 3 values per line) which specify the grain orientations. Each vector is a displacement from a central atom (0,0,0) to a nearest neighbor atom in an fcc lattice at the proper orientation. The vector lengths should all be identical since an fcc lattice has a coordination number of 12. Only 6 are listed due to symmetry, so the list must include one from each pair of equal-and-opposite neighbors. A pair of orientation files for a Sigma=5 tilt boundary are shown below. A tutorial that can help for writing the orientation files is given in *(Wicaksono2)*

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify energy* option is supported by this fix to add the potential energy of atom interactions with the grain boundary driving force to the system's potential energy as part of *thermodynamic output*.

The *fix_modify respa* option is supported by these fixes. This allows to set at which level of the *r-RESPA* integrator a fix is adding its forces. Default is the outermost level.

This fix calculates a global scalar which can be accessed by various *output commands*. The scalar is the potential energy change due to this fix. The scalar value calculated by this fix is "extensive".

This fix also calculates a per-atom array which can be accessed by various *output commands*. The array stores the order parameter Xi and normalized order parameter (0 to 1) for each atom. The per-atom values can be accessed on any timestep.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.158.3 Restrictions

This fix is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix should only be used with fcc or bcc lattices.

16.158.4 Related commands

fix_modify

Default: none

(Janssens) Janssens, Olmsted, Holm, Foiles, Plimpton, Derlet, Nature Materials, 5, 124-127 (2006).

(Wicaksono1) Wicaksono, Sinclair, Militzer, Computational Materials Science, 117, 397-405 (2016).

(Wicaksono2) Wicaksono, figshare, https://dx.doi.org/10.6084/m9.figshare.1488628.v1 (2015).

For illustration purposes, here are example files that specify a Sigma=5 <100> tilt boundary. This is for a lattice constant of 3.5706 Angs.

file0:

```
 0.798410432046075    1.785300000000000    1.596820864092150
-0.798410432046075    1.785300000000000   -1.596820864092150
 2.395231296138225    0.000000000000000    0.798410432046075
 0.798410432046075    0.000000000000000   -2.395231296138225
 1.596820864092150    1.785300000000000   -0.798410432046075
 1.596820864092150   -1.785300000000000   -0.798410432046075
```

file1:

```
-0.798410432046075    1.785300000000000    1.596820864092150
 0.798410432046075    1.785300000000000   -1.596820864092150
 0.798410432046075    0.000000000000000    2.395231296138225
 2.395231296138225    0.000000000000000   -0.798410432046075
 1.596820864092150    1.785300000000000    0.798410432046075
 1.596820864092150   -1.785300000000000    0.798410432046075
```

16.159 fix phonon command

16.159.1 Syntax

```
fix ID group-ID phonon N Noutput Nwait map_file prefix keyword values ...
```

- ID, group-ID are documented in *fix* command
- phonon = style name of this fix command
- N = measure the Green's function every this many timesteps
- Noutput = output the dynamical matrix every this many measurements

- Nwait = wait this many timesteps before measuring
- map_file = *file* or *GAMMA*

```
file is the file that contains the mapping info between atom ID and the␣
↪lattice indices.

GAMMA flags to treate the whole simulation box as a unit cell, so that␣
↪the mapping
info can be generated internally. In this case, dynamical matrix at only␣
↪the gamma-point
will/can be evaluated.
```

- prefix = prefix for output files
- one or none keyword/value pairs may be appended
- keyword = *sysdim* or *nasr*

```
sysdim value = d
  d = dimension of the system, usually the same as the MD model dimension
nasr value = n
  n = number of iterations to enforce the acoustic sum rule
```

16.159.2 Examples

```
fix 1 all phonon 20 5000 200000 map.in LJ1D sysdim 1
fix 1 all phonon 20 5000 200000 map.in EAM3D
fix 1 all phonon 10 5000 500000 GAMMA EAM0D nasr 100
```

16.159.3 Description

Calculate the dynamical matrix from molecular dynamics simulations based on fluctuation-dissipation theory for a group of atoms.

Consider a crystal with N unit cells in three dimensions labeled $l = (l_1, l_2, l_3)$ where l_i are integers. Each unit cell is defined by three linearly independent vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ forming a parallelepiped, containing K basis atoms labeled k.

Based on fluctuation-dissipation theory, the force constant coefficients of the system in reciprocal space are given by (*Campana* , *Kong*)

$$\mathbf{\Phi}_{k\alpha,k'\beta}(\mathbf{q}) = k_B T \mathbf{G}^{-1}_{k\alpha,k'\beta}(\mathbf{q})$$

where $\mathbf{G}$ is the Green's functions coefficients given by

$$\mathbf{G}_{k\alpha,k'\beta}(\mathbf{q}) = \left\langle \mathbf{u}_{k\alpha}(\mathbf{q}) \bullet \mathbf{u}^*_{k'\beta}(\mathbf{q}) \right\rangle$$

where $\langle \ldots \rangle$ denotes the ensemble average, and

$$\mathbf{u}_{k\alpha}(\mathbf{q}) = \sum_l \mathbf{u}_{lk\alpha} \exp\left(i\mathbf{q}\mathbf{r}_l\right)$$

is the α component of the atomic displacement for the k th atom in the unit cell in reciprocal space at $\mathbf{q}$. In practice, the Green's functions coefficients can also be measured according to the following formula,

$$\mathbf{G}_{k\alpha,k'\beta}(\mathbf{q}) = \left\langle \mathbf{R}_{k\alpha}(\mathbf{q}) \bullet \mathbf{R}^*_{k'\beta}(\mathbf{q}) \right\rangle - \left\langle \mathbf{R} \right\rangle_{k\alpha}(\mathbf{q}) \bullet \left\langle \mathbf{R} \right\rangle^*_{k'\beta}(\mathbf{q})$$

where $\mathbf{R}$ is the instantaneous positions of atoms, and $\langle \mathbf{R} \rangle$ is the averaged atomic positions. It gives essentially the same results as the displacement method and is easier to implement in an MD code.

Once the force constant matrix is known, the dynamical matrix $\mathbf{D}$ can then be obtained by

$$\mathbf{D}_{k\alpha,k'\beta}(\mathbf{q}) = (m_k m_{k'})^{-\frac{1}{2}} \mathbf{\Phi}_{k\alpha,k'\beta}(\mathbf{q})$$

whose eigenvalues are exactly the phonon frequencies at $\mathbf{q}$.

This fix uses positions of atoms in the specified group and calculates two-point correlations. To achieve this. the positions of the atoms are examined every *Nevery* steps and are Fourier-transformed into reciprocal space, where the averaging process and correlation computation is then done. After every *Noutput* measurements, the matrix $\mathbf{G}(\mathbf{q})$ is calculated and inverted to obtain the elastic stiffness coefficients. The dynamical matrices are then constructed and written to *prefix*.bin.timestep files in binary format and to the file *prefix*.log for each wave-vector $\mathbf{q}$.

A detailed description of this method can be found in (*Kong2011*).

The *sysdim* keyword is optional. If specified with a value smaller than the dimensionality of the LAMMPS simulation, its value is used for the dynamical matrix calculation. For example, using LAMMPS ot model a 2D or 3D system, the phonon dispersion of a 1D atomic chain can be computed using *sysdim* = 1.

The *nasr* keyword is optional. An iterative procedure is employed to enforce the acoustic sum rule on Φ at Γ, and the number provided by keyword *nasr* gives the total number of iterations. For a system whose unit cell has only one atom, *nasr* = 1 is sufficient; for other systems, *nasr* = 10 is typically sufficient.

The *map_file* contains the mapping information between the lattice indices and the atom IDs, which tells the code which atom sits at which lattice point; the lattice indices start from 0. An auxiliary code, latgen, can be employed to generate the compatible map file for various crystals.

In case one simulates a non-periodic system, where the whole simulation box is treated as a unit cell, one can set *map_file* as *GAMMA*, so that the mapping info will be generated internally and a file is not needed. In this case, the dynamical matrix at only the gamma-point will/can be evaluated. Please keep in mind that fix-phonon is designed for cyrstals, it will be inefficient and even degrade the performance of lammps in case the unit cell is too large.

The calculated dynamical matrix elements are written out in *energy/distance^2/mass* units. The coordinates for *q* points in the log file is in the units of the basis vectors of the corresponding reciprocal lattice.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify temp* option is supported by this fix. You can use it to change the temperature compute from thermo_temp to the one that reflects the true temperature of atoms in the group.

No global scalar or vector or per-atom quantities are stored by this fix for access by various *output commands*.

Instead, this fix outputs its initialization information (including mapping information) and the calculated dynamical matrices to the file *prefix*.log, with the specified *prefix*. The dynamical matrices are also written to files *prefix*.bin.timestep in binary format. These can be read by the post-processing tool in tools/phonon to compute the phonon density of states and/or phonon dispersion curves.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

This fix is not invoked during *energy minimization*.

16.159.4 Restrictions

This fix assumes a crystalline system with periodical lattice. The temperature of the system should not exceed the melting temperature to keep the system in its solid state.

This fix is part of the USER-PHONON package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix requires LAMMPS be built with an FFT library. See the *Build settings* doc page for details.

16.159.5 Related commands

compute msd, *dynamical_matrix*

16.159.6 Default

The option defaults are sysdim = the same dimension as specified by the *dimension* command, and nasr = 20.

(Campana) C. Campana and M. H. Muser, *Practical Green's function approach to the simulation of elastic semi-infinite solids*, Phys. Rev. B [74], 075420 (2006)

(Kong) L.T. Kong, G. Bartels, C. Campana, C. Denniston, and Martin H. Muser, *Implementation of Green's function molecular dynamics: An extension to LAMMPS*, Computer Physics Communications [180](6):1004-1010 (2009).

L.T. Kong, C. Denniston, and Martin H. Muser, *An improved version of the Green's function molecular dynamics method*, Computer Physics Communications [182](2):540-541 (2011).

(Kong2011) L.T. Kong, *Phonon dispersion measured directly from molecular dynamics simulations*, Computer Physics Communications [182](10):2201-2207, (2011).

16.160 fix pimd command

16.160.1 Syntax

```
fix ID group-ID pimd keyword value ...
```

- ID, group-ID are documented in *fix* command
- pimd = style name of this fix command
- zero or more keyword/value pairs may be appended
- keyword = *method* or *fmass* or *sp* or *temp* or *nhc*

```
method value = pimd or nmpimd or cmd
fmass value = scaling factor on mass
sp value = scaling factor on Planck constant
temp value = temperature (temperarate units)
nhc value = Nc = number of chains in Nose-Hoover thermostat
```

16.160.2 Examples

```
fix 1 all pimd method nmpimd fmass 1.0 sp 2.0 temp 300.0 nhc 4
```

16.160.3 Description

This command performs quantum molecular dynamics simulations based on the Feynman path integral to include effects of tunneling and zero-point motion. In this formalism, the isomorphism of a quantum partition function for the original system to a classical partition function for a ring-polymer system is exploited, to efficiently sample configurations from the canonical ensemble *(Feynman)*. The classical partition function and its components are given by the following equations:

$$Z = \int d\mathbf{q} d\mathbf{p} \cdot \exp[-\beta H_{eff}]$$

$$H_{eff} = \left(\sum_{i=1}^{P} \frac{p_i^2}{2m_i} \right) + V_{eff}$$

$$V_{eff} = \sum_{i=1}^{P} \left[\frac{mP}{2\beta^2\hbar^2}(q_i - q_{i+1})^2 + \frac{1}{P}V(q_i) \right]$$

The interested user is referred to any of the numerous references on this methodology, but briefly, each quantum particle in a path integral simulation is represented by a ring-polymer of P quasi-beads, labeled from 1 to P. During the simulation, each quasi-bead interacts with beads on the other ring-polymers with the same imaginary time index (the second term in the effective potential above). The quasi-beads also interact with the two neighboring quasi-beads through the spring potential in imaginary-time space (first term in effective potential). To sample the canonical ensemble, a Nose-Hoover massive chain thermostat is applied *(Tuckerman)*. With the massive chain algorithm, a chain of NH thermostats is coupled to each degree of freedom for each quasi-bead. The keyword *temp* sets the target temperature for the system and the keyword *nhc* sets the number *Nc* of thermostats in each chain. For example, for a simulation of N particles with P beads in each ring-polymer, the total number of NH thermostats would be 3 x N x P x Nc.

Note: This fix implements a complete velocity-verlet integrator combined with NH massive chain thermostat, so no other time integration fix should be used.

The *method* keyword determines what style of PIMD is performed. A value of *pimd* is standard PIMD. A value of *nmpimd* is for normal-mode PIMD. A value of *cmd* is for centroid molecular dynamics (CMD). The difference between the styles is as follows.

In standard PIMD, the value used for a bead's fictitious mass is arbitrary. A common choice is to use Mi = m/P, which results in the mass of the entire ring-polymer being equal to the real quantum particle. But it can be difficult to efficiently integrate the equations of motion for the stiff harmonic interactions in the ring polymers.

A useful way to resolve this issue is to integrate the equations of motion in a normal mode representation, using Normal Mode Path-Integral Molecular Dynamics (NMPIMD) *(Cao1)*. In NMPIMD, the NH chains are attached to each normal mode of the ring-polymer and the fictitious mass of each mode is chosen as Mk = the eigenvalue of the Kth normal mode for k > 0. The k = 0 mode, referred to as the zero-frequency mode or centroid, corresponds to overall translation of the ring-polymer and is assigned the mass of the real particle.

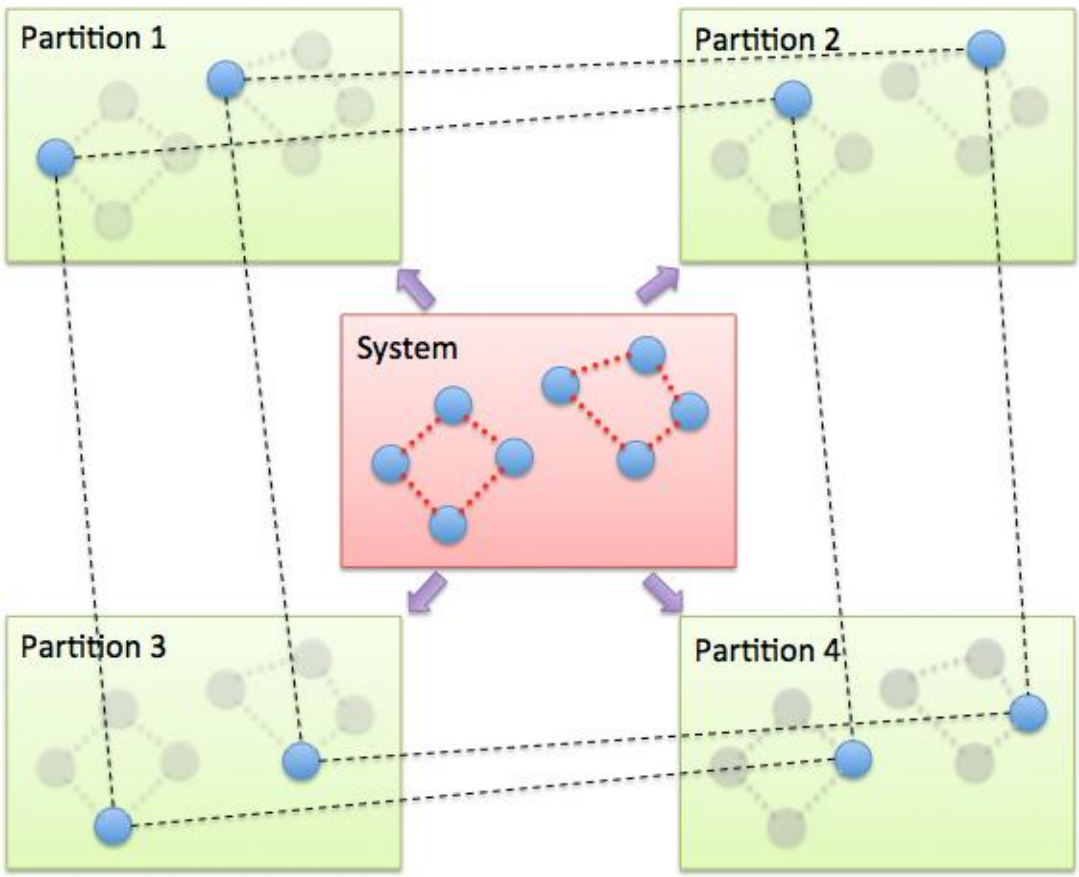
Motion of the centroid can be effectively uncoupled from the other normal modes by scaling the fictitious masses to achieve a partial adiabatic separation. This is called a Centroid Molecular Dynamics (CMD) approximation *(Cao2)*. The time-evolution (and resulting dynamics) of the quantum particles can be used to obtain centroid time correlation functions, which can be further used to obtain the true quantum correlation function for the original system. The CMD

method also uses normal modes to evolve the system, except only the k > 0 modes are thermostatted, not the centroid degrees of freedom.

The keyword *fmass* sets a further scaling factor for the fictitious masses of beads, which can be used for the Partial Adiabatic CMD *(Hone)*, or to be set as P, which results in the fictitious masses to be equal to the real particle masses.

The keyword *sp* is a scaling factor on Planck's constant, which can be useful for debugging or other purposes. The default value of 1.0 is appropriate for most situations.

The PIMD algorithm in LAMMPS is implemented as a hyper-parallel scheme as described in *(Calhoun)*. In LAMMPS this is done by using *multi-replica feature* in LAMMPS, where each quasi-particle system is stored and simulated on a separate partition of processors. The following diagram illustrates this approach. The original system with 2 ring polymers is shown in red. Since each ring has 4 quasi-beads (imaginary time slices), there are 4 replicas of the system, each running on one of the 4 partitions of processors. Each replica (shown in green) owns one quasi-bead in each ring.



To run a PIMD simulation with M quasi-beads in each ring polymer using N MPI tasks for each partition's domain-decomposition, you would use P = MxN processors (cores) and run the simulation as follows:

```
mpirun -np P lmp_mpi -partition MxN -in script
```

Note that in the LAMMPS input script for a multi-partition simulation, it is often very useful to define a *uloop-style variable* such as

```
variable ibead uloop M pad
```

where M is the number of quasi-beads (partitions) used in the calculation. The uloop variable can then be used to manage I/O related tasks for each of the partitions, e.g.

```
dump dcd all dcd 10 system_${ibead}.dcd
restart 1000 system_${ibead}.restart1 system_${ibead}.restart2
read_restart system_${ibead}.restart2
```

16.160.4 Restrictions

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

A PIMD simulation can be initialized with a single data file read via the *read_data* command. However, this means all quasi-beads in a ring polymer will have identical positions and velocities, resulting in identical trajectories for all quasi-beads. To avoid this, users can simply initialize velocities with different random number seeds assigned to each partition, as defined by the uloop variable, e.g.

```
velocity all create 300.0 1234${ibead} rot yes dist gaussian
```

16.160.5 Default

The keyword defaults are method = pimd, fmass = 1.0, sp = 1.0, temp = 300.0, and nhc = 2.

(Feynman) R. Feynman and A. Hibbs, Chapter 7, Quantum Mechanics and Path Integrals, McGraw-Hill, New York (1965).

(Tuckerman) M. Tuckerman and B. Berne, J Chem Phys, 99, 2796 (1993).

(Cao1) J. Cao and B. Berne, J Chem Phys, 99, 2902 (1993).

(Cao2) J. Cao and G. Voth, J Chem Phys, 100, 5093 (1994).

(Hone) T. Hone, P. Rossky, G. Voth, J Chem Phys, 124, 154103 (2006).

(Calhoun) A. Calhoun, M. Pavese, G. Voth, Chem Phys Letters, 262, 415 (1996).

16.161 fix planeforce command

16.161.1 Syntax

```
fix ID group-ID planeforce x y z
```

- ID, group-ID are documented in *fix* command
- planeforce = style name of this fix command
- x y z = 3-vector that is normal to the plane

16.161.2 Examples

```
fix hold boundary planeforce 1.0 0.0 0.0
```

16.161.3 Description

Adjust the forces on each atom in the group so that only the components of force in the plane specified by the normal vector (x,y,z) remain. This is done by subtracting out the component of force perpendicular to the plane.

If the initial velocity of the atom is 0.0 (or in the plane), then it should continue to move in the plane thereafter.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command.

16.161.4 Restrictions

none

16.161.5 Related commands

fix lineforce

Default: none

16.162 fix plumed command

16.162.1 Syntax

```
fix ID group-ID plumed keyword value ...
```

- ID, group-ID are documented in *fix* command
- plumed = style name of this fix command
- keyword = *plumedfile* or *outfile*

```
plumedfile arg = name of PLUMED input file to use (default: NULL)
outfile arg = name of file on which to write the PLUMED log (default:
↪NULL)
```

16.162.2 Examples

fix pl all plumed all plumed plumedfile plumed.dat outfile p.log

16.162.3 Description

This fix instructs LAMMPS to call the PLUMED library, which allows one to perform various forms of trajectory analysis on the fly and to also use methods such as umbrella sampling and metadynamics to enhance the sampling of phase space.

The documentation included here only describes the fix plumed command itself. This command is LAMMPS specific, whereas most of the functionality implemented in PLUMED will work with a range of MD codes, and when PLUMED is used as a stand alone code for analysis. The full documentation for PLUMED is available online and included in the PLUMED source code. The PLUMED library development is hosted at https://github.com/plumed/plumed2 A detailed discussion of the code can be found in *(PLUMED)*.

There is an example input for using this package with LAMMPS in the examples/USER/plumed directory.

The command to make LAMMPS call PLUMED during a run requires two keyword value pairs pointing to the PLUMED input file and an output file for the PLUMED log. The user must specify these arguments every time PLUMED is to be used. Furthermore, the fix plumed command should appear in the LAMMPS input file **after** relevant input parameters (e.g. the timestep) have been set.

The *group-ID* entry is ignored. LAMMPS will always pass all the atoms to PLUMED and there can only be one instance of the plumed fix at a time. The way the plumed fix is implemented ensures that the minimum amount of information required is communicated. Furthermore, PLUMED supports multiple, completely independent collective variables, multiple independent biases and multiple independent forms of analysis. There is thus really no restriction in functionality by only allowing only one plumed fix in the LAMMPS input.

The *plumedfile* keyword allows the user to specify the name of the PLUMED input file. Instructions as to what should be included in a plumed input file can be found in the documentation for PLUMED

The *outfile* keyword allows the user to specify the name of a file in which to output the PLUMED log. This log file normally just repeats the information that is contained in the input file to confirm it was correctly read and parsed. The names of the files in which the results are stored from the various analysis options performed by PLUMED will be specified by the user in the PLUMED input file.

Restart, fix_modify, output, run start/stop, minimize info:

When performing a restart of a calculation that involves PLUMED you must include a RESTART command in the PLUMED input file as detailed in the PLUMED documentation. When the restart command is found in the PLUMED input PLUMED will append to the files that were generated in the run that was performed previously. No part of the PLUMED restart data is included in the LAMMPS restart files. Furthermore, any history dependent bias potentials that were accumulated in previous calculations will be read in when the RESTART command is included in the PLUMED input.

The *fix_modify* *energy* option is not supported by this fix.

Nothing is computed by this fix that can be accessed by any of the *output commands* within LAMMPS. All the quantities of interest can be output by commands that are native to PLUMED, however.

16.162.4 Restrictions

This fix is part of the USER-PLUMED package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

There can only be one plumed fix active at a time.

16.162.5 Related commands

fix smd fix colvars

16.162.6 Default

The default options are plumedfile = NULL and outfile = NULL

(PLUMED) G.A. Tribello, M. Bonomi, D. Branduardi, C. Camilloni and G. Bussi, Comp. Phys. Comm 185, 604 (2014)

16.163 fix poems command

Syntax:

```
fix ID group-ID poems keyword values
```

- ID, group-ID are documented in *fix* command
- poems = style name of this fix command
- keyword = *group* or *file* or *molecule*

  ```
  group values = list of group IDs
  molecule values = none
  file values = filename
  ```

16.163.1 Examples

```
fix 3 fluid poems group clump1 clump2 clump3
fix 3 fluid poems file cluster.list
```

16.163.2 Description

Treats one or more sets of atoms as coupled rigid bodies. This means that each timestep the total force and torque on each rigid body is computed and the coordinates and velocities of the atoms are updated so that the collection of bodies move as a coupled set. This can be useful for treating a large biomolecule as a collection of connected, coarse-grained particles.

The coupling, associated motion constraints, and time integration is performed by the software package Parallelizable Open source Efficient Multibody Software (POEMS) which computes the constrained rigid-body motion of articulated (jointed) multibody systems *(Anderson)*. POEMS was written and is distributed by Prof Kurt Anderson, his graduate

student Rudranarayan Mukherjee, and other members of his group at Rensselaer Polytechnic Institute (RPI). Rudranarayan developed the LAMMPS/POEMS interface. For copyright information on POEMS and other details, please refer to the documents in the poems directory distributed with LAMMPS.

This fix updates the positions and velocities of the rigid atoms with a constant-energy time integration, so you should not update the same atoms via other fixes (e.g. nve, nvt, npt, temp/rescale, langevin).

Each body must have a non-degenerate inertia tensor, which means if must contain at least 3 non-collinear atoms. Which atoms are in which bodies can be defined via several options.

For option *group*, each of the listed groups is treated as a rigid body. Note that only atoms that are also in the fix group are included in each rigid body.

For option *molecule*, each set of atoms in the group with a different molecule ID is treated as a rigid body.

For option *file*, sets of atoms are read from the specified file and each set is treated as a rigid body. Each line of the file specifies a rigid body in the following format:

ID type atom1-ID atom2-ID atom3-ID . . .

ID as an integer from 1 to M (the number of rigid bodies). Type is any integer; it is not used by the fix poems command. The remaining arguments are IDs of atoms in the rigid body, each typically from 1 to N (the number of atoms in the system). Only atoms that are also in the fix group are included in each rigid body. Blank lines and lines that begin with '#' are skipped.

A connection between a pair of rigid bodies is inferred if one atom is common to both bodies. The POEMS solver treats that atom as a spherical joint with 3 degrees of freedom. Currently, a collection of bodies can only be connected by joints as a linear chain. The entire collection of rigid bodies can represent one or more chains. Other connection topologies (tree, ring) are not allowed, but will be added later. Note that if no joints exist, it is more efficient to use the *fix rigid* command to simulate the system.

When the poems fix is defined, it will print out statistics on the total # of clusters, bodies, joints, atoms involved. A cluster in this context means a set of rigid bodies connected by joints.

For computational efficiency, you should turn off pairwise and bond interactions within each rigid body, as they no longer contribute to the motion. The "neigh_modify exclude" and "delete_bonds" commands can be used to do this if each rigid body is a group.

For computational efficiency, you should only define one fix poems which includes all the desired rigid bodies. LAMMPS will allow multiple poems fixes to be defined, but it is more expensive.

The degrees-of-freedom removed by coupled rigid bodies are accounted for in temperature and pressure computations. Similarly, the rigid body contribution to the pressure virial is also accounted for. The latter is only correct if forces within the bodies have been turned off, and there is only a single fix poems defined.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify* *bodyforces* option is supported by this fix style to set whether per-body forces and torques are computed early or late in a timestep, i.e. at the post-force stage or at the final-integrate stage, respectively.

No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.163.3 Restrictions

This fix is part of the POEMS package. It is only enabled if LAMMPS was built with that package, which also requires the POEMS library be built and linked with LAMMPS. See the *Build package* doc page for more info.

16.163.4 Related commands

fix rigid, *delete_bonds*, *neigh_modify* exclude

Default: none

(Anderson) Anderson, Mukherjee, Critchley, Ziegler, and Lipton "POEMS: Parallelizable Open-source Efficient Multibody Software ", Engineering With Computers (2006). (link to paper)

16.164 fix pour command

16.164.1 Syntax

```
fix ID group-ID pour N type seed keyword values ...
```

- ID, group-ID are documented in *fix* command
- pour = style name of this fix command
- N = # of particles to insert
- type = atom type to assign to inserted particles (offset for molecule insertion)
- seed = random # seed (positive integer)
- one or more keyword/value pairs may be appended to args
- keyword = *region* or *diam* or *vol* or *rate* or *dens* or *vel* or *mol* or *rigid* or *shake* or *ignore*

```
region value = region-ID
  region-ID = ID of region to use as insertion volume
diam values = dstyle args
  dstyle = one or range or poly
    one args = D
      D = single diameter for inserted particles (distance units)
    range args = Dlo Dhi
      Dlo,Dhi = range of diameters for inserted particles (distance units)
    poly args = Npoly D1 P1 D2 P2 ...
      Npoly = # of (D,P) pairs
      D1,D2,... = diameter for subset of inserted particles (distance␣
↪units)
      P1,P2,... = percentage of inserted particles with this diameter␣
↪(0-1)
id values = idflag
  idflag = max or next = how to choose IDs for inserted particles and␣
↪molecules
vol values = fraction Nattempt
  fraction = desired volume fraction for filling insertion volume
  Nattempt = max # of insertion attempts per particle
```

```
rate value = V
  V = z velocity (3d) or y velocity (2d) at which
      insertion volume moves (velocity units)
dens values = Rholo Rhohi
  Rholo,Rhohi = range of densities for inserted particles (mass/volume␣
↪units)
vel values (3d) = vxlo vxhi vylo vyhi vz
vel values (2d) = vxlo vxhi vy
  vxlo,vxhi = range of x velocities for inserted particles (velocity␣
↪units)
  vylo,vyhi = range of y velocities for inserted particles (velocity␣
↪units)
  vz = z velocity (3d) assigned to inserted particles (velocity units)
  vy = y velocity (2d) assigned to inserted particles (velocity units)
mol value = template-ID
  template-ID = ID of molecule template specified in a separate molecule␣
↪command
molfrac values = f1 f2 ... fN
  f1 to fN = relative probability of creating each of N molecules in␣
↪template-ID
rigid value = fix-ID
  fix-ID = ID of fix rigid/small command
shake value = fix-ID
  fix-ID = ID of fix shake command
ignore value = none
  skip any line or triangle particles when detecting possible
    overlaps with inserted particles
```

16.164.2 Examples

```
fix 3 all pour 1000 2 29494 region myblock
fix 2 all pour 10000 1 19985583 region disk vol 0.33 100 rate 1.0 diam range 0.9 1.1
fix 2 all pour 10000 1 19985583 region disk diam poly 2 0.7 0.4 1.5 0.6
fix ins all pour 500 1 4767548 vol 0.8 10 region slab mol object rigid myRigid
```

16.164.3 Description

Insert finite-size particles or molecules into the simulation box every few timesteps within a specified region until N particles or molecules have been inserted. This is typically used to model the pouring of granular particles into a container under the influence of gravity. For the remainder of this doc page, a single inserted atom or molecule is referred to as a "particle".

If inserted particles are individual atoms, they are assigned the specified atom type. If they are molecules, the type of each atom in the inserted molecule is specified in the file read by the *molecule* command, and those values are added to the specified atom type. E.g. if the file specifies atom types 1,2,3, and those are the atom types you want for inserted molecules, then specify *type* = 0. If you specify *type* = 2, the in the inserted molecule will have atom types 3,4,5.

All atoms in the inserted particle are assigned to two groups: the default group "all" and the group specified in the fix pour command (which can also be "all").

This command must use the *region* keyword to define an insertion volume. The specified region must have been previously defined with a *region* command. It must be of type *block* or a z-axis *cylinder* and must be defined with side = *in*. The cylinder style of region can only be used with 3d simulations.

Individual atoms are inserted, unless the *mol* keyword is used. It specifies a *template-ID* previously defined using the *molecule* command, which reads a file that defines the molecule. The coordinates, atom types, center-of-mass, moments of inertia, etc, as well as any bond/angle/etc and special neighbor information for the molecule can be specified in the molecule file. See the *molecule* command for details. The only settings required to be in this file are the coordinates and types of atoms in the molecule.

If the molecule template contains more than one molecule, the relative probability of depositing each molecule can be specified by the *molfrac* keyword. N relative probabilities, each from 0.0 to 1.0, are specified, where N is the number of molecules in the template. Each time a molecule is inserted, a random number is used to sample from the list of relative probabilities. The N values must sum to 1.0.

If you wish to insert molecules via the *mol* keyword, that will be treated as rigid bodies, use the *rigid* keyword, specifying as its value the ID of a separate *fix rigid/small* command which also appears in your input script.

Note: If you wish the new rigid molecules (and other rigid molecules) to be thermostatted correctly via *fix rigid/small/nvt* or *fix rigid/small/npt*, then you need to use the "fix_modify dynamic/dof yes" command for the rigid fix. This is to inform that fix that the molecule count will vary dynamically.

If you wish to insert molecules via the *mol* keyword, that will have their bonds or angles constrained via SHAKE, use the *shake* keyword, specifying as its value the ID of a separate *fix shake* command which also appears in your input script.

Each timestep particles are inserted, they are placed randomly inside the insertion volume so as to mimic a stream of poured particles. If they are molecules they are also oriented randomly. Each atom in the particle is tested for overlaps with existing particles, including effects due to periodic boundary conditions if applicable. If an overlap is detected, another random insertion attempt is made; see the *vol* keyword discussion below. The larger the volume of the insertion region, the more particles that can be inserted at any one timestep. Particles are inserted again after enough time has elapsed that the previously inserted particles fall out of the insertion volume under the influence of gravity. Insertions continue every so many timesteps until the desired # of particles has been inserted.

Note: If you are monitoring the temperature of a system where the particle count is changing due to adding particles, you typically should use the *compute_modify dynamic yes* command for the temperature compute you are using.

All other keywords are optional with defaults as shown below.

The *diam* option is only used when inserting atoms and specifies the diameters of inserted particles. There are 3 styles: *one*, *range*, or *poly*. For *one*, all particles will have diameter *D*. For *range*, the diameter of each particle will be chosen randomly and uniformly between the specified *Dlo* and *Dhi* bounds. For *poly*, a series of *Npoly* diameters is specified. For each diameter a percentage value from 0.0 to 1.0 is also specified. The *Npoly* percentages must sum to 1.0. For the example shown above with "diam 2 0.7 0.4 1.5 0.6", all inserted particles will have a diameter of 0.7 or 1.5. 40% of the particles will be small; 60% will be large.

Note that for molecule insertion, the diameters of individual atoms in the molecule can be specified in the file read by the *molecule* command. If not specified, the diameter of each atom in the molecule has a default diameter of 1.0.

The *id* option has two settings which are used to determine the atom or molecule IDs to assign to inserted particles/molecules. In both cases a check is done of the current system to find the maximum current atom and molecule ID of any existing particle. Newly inserted particles and molecules are assigned IDs that increment those max values. For the *max* setting, which is the default, this check is done at every insertion step, which allows for particles to leave the system, and their IDs to potentially be re-used. For the *next* setting this check is done only once when the fix is specified, which can be more efficient if you are sure particles will not be added in some other way.

The *vol* option specifies what volume fraction of the insertion volume will be filled with particles. For particles with a size specified by the *diam range* keyword, they are assumed to all be of maximum diameter *Dhi* for purposes of

computing their contribution to the volume fraction.

The higher the volume fraction value, the more particles are inserted each timestep. Since inserted particles cannot overlap, the maximum volume fraction should be no higher than about 0.6. Each timestep particles are inserted, LAMMPS will make up to a total of M tries to insert the new particles without overlaps, where M = # of inserted particles * Nattempt. If LAMMPS is unsuccessful at completing all insertions, it prints a warning.

The *dens* and *vel* options enable inserted particles to have a range of densities or xy velocities. The specific values for a particular inserted particle will be chosen randomly and uniformly between the specified bounds. Internally, the density value for a particle is converted to a mass, based on the radius (volume) of the particle. The *vz* or *vy* value for option *vel* assigns a z-velocity (3d) or y-velocity (2d) to each inserted particle.

The *rate* option moves the insertion volume in the z direction (3d) or y direction (2d). This enables pouring particles from a successively higher height over time.

The *ignore* option is useful when running a simulation that used line segment (2d) or triangle (3d) particles, typically to define boundaries for spherical granular particles to interact with. See the *atom_style line or tri* command for details. Lines and triangles store their size, and if the size is large it may overlap (in a spherical sense) with the insertion region, even if the line/triangle is oriented such that there is no actual overlap. This can prevent particles from being inserted. The *ignore* keyword causes the overlap check to skip any line or triangle particles. Obviously you should only use it if there is in fact no overlap of the line or triangle particles with the insertion region.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. This means you must be careful when restarting a pouring simulation, when the restart file was written in the middle of the pouring operation. Specifically, you should use a new fix pour command in the input script for the restarted simulation that continues the operation. You will need to adjust the arguments of the original fix pour command to do this.

Also note that because the state of the random number generator is not saved in restart files, you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior if you adjust the fix pour parameters appropriately.

None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.164.4 Restrictions

This fix is part of the GRANULAR package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

For 3d simulations, a gravity fix in the -z direction must be defined for use in conjunction with this fix. For 2d simulations, gravity must be defined in the -y direction.

The specified insertion region cannot be a "dynamic" region, as defined by the *region* command.

16.164.5 Related commands

fix deposit, *fix gravity*, *region*

16.164.6 Default

Insertions are performed for individual particles, i.e. no *mol* setting is defined. If the *mol* keyword is used, the default for *molfrac* is an equal probabilities for all molecules in the template. Additional option defaults are diam = one 1.0, dens = 1.0 1.0, vol = 0.25 50, rate = 0.0, vel = 0.0 0.0 0.0 0.0 0.0 (for 3d), vel = 0.0 0.0 0.0 (for 2d), and id = max.

16.165 fix precession/spin command

16.165.1 Syntax

```
fix ID group precession/spin style args
```

- ID, group are documented in *fix* command
- precession/spin = style name of this fix command
- style = *zeeman* or *anisotropy* or *cubic*

```
zeeman args = H x y z
  H = intensity of the magnetic field (in Tesla)
  x y z = vector direction of the field
anisotropy args = K x y z
  K = intensity of the magnetic anisotropy (in eV)
  x y z = vector direction of the anisotropy

cubic args = K1 K2c n1x n1y n1x n2x n2y n2z n3x n3y n3z
  K1 and K2c = intensity of the magnetic anisotropy (in eV)
  n1x to n3z = three direction vectors of the cubic anisotropy
```

16.165.2 Examples

```
fix 1 all precession/spin zeeman 0.1 0.0 0.0 1.0
fix 1 3 precession/spin anisotropy 0.001 0.0 0.0 1.0
fix 1 iron precession/spin cubic 0.001 0.0005 1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0
fix 1 all precession/spin zeeman 0.1 0.0 0.0 1.0 anisotropy 0.001 0.0 0.0 1.0
```

16.165.3 Description

This fix applies a precession torque to each magnetic spin in the group.

Style *zeeman* is used for the simulation of the interaction between the magnetic spins in the defined group and an external magnetic field:

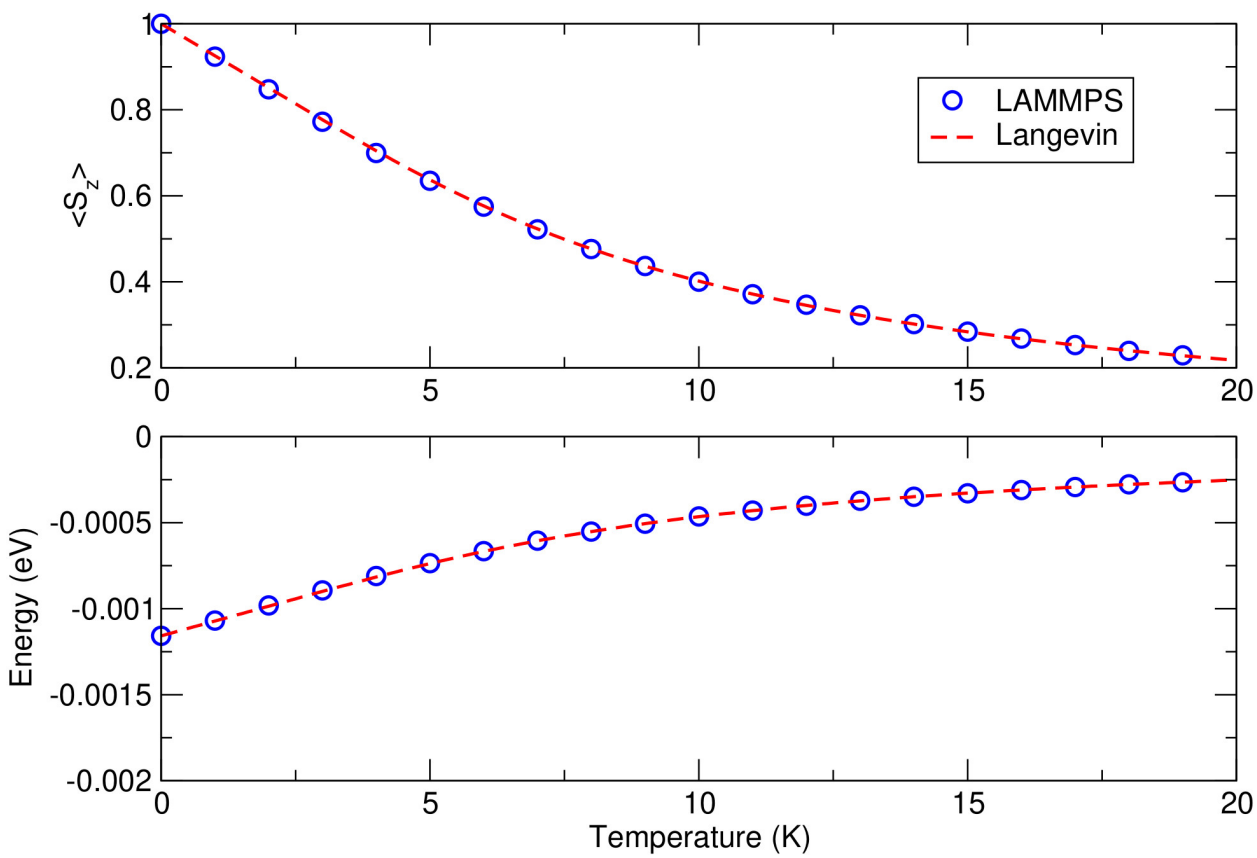
$$H_{Zeeman} = -g \sum_{i=0}^{N} \mu_i \, \vec{s}_i \cdot \vec{B}_{ext}$$

with:

- $\vec{B}_{ext}$ the external magnetic field (in T)
- g the Lande factor (hard-coded as $g = 2.0$)
- $\vec{s}_i$ the unitary vector describing the orientation of spin i
- μ_i the atomic moment of spin i given as a multiple of the Bohr magneton μ_B (for example, $\mu_i \approx 2.2$ in bulk iron).

The field value in Tesla is multiplied by the gyromagnetic ratio, $g \cdot \mu_B/\hbar$, converting it into a precession frequency in rad.THz (in metal units and with $\mu_B = 5.788eV/T$).

As a comparison, the figure below displays the simulation of a single spin (of norm $\mu_i = 1.0$) submitted to an external magnetic field of $|B_{ext}| = 10.0$ Tesla (and oriented along the z axis). The upper plot shows the average magnetization along the external magnetic field axis and the lower plot the Zeeman energy, both as a function of temperature. The reference result is provided by the plot of the Langevin function for the same parameters.



The temperature effects are accounted for by connecting the spin i to a thermal bath using a Langevin thermostat (see *fix langevin/spin* for the definition of this thermostat).

Style *anisotropy* is used to simulate an easy axis or an easy plane for the magnetic spins in the defined group:

$$H_{aniso} = -\sum_{i=1}^{N} K_{an}(\mathbf{r}_i)\ (\vec{s}_i \cdot \vec{n}_i)^2$$

with n defining the direction of the anisotropy, and K (in eV) its intensity. If $K > 0$, an easy axis is defined, and if $K < 0$, an easy plane is defined.

Style *cubic* is used to simulate a cubic anisotropy, with three possible easy axis for the magnetic spins in the defined

group:

$$H_{cubic} = -\sum_{i=1}^{N} K_1 \left[(\vec{s}_i \cdot \vec{n_1})^2 (\vec{s}_i \cdot \vec{n_2})^2 + (\vec{s}_i \cdot \vec{n_2})^2 (\vec{s}_i \cdot \vec{n_3})^2 + (\vec{s}_i \cdot \vec{n_1})^2 (\vec{s}_i \cdot \vec{n_3})^2 \right] + K_2^{(c)} (\vec{s}_i \cdot \vec{n_1})^2 (\vec{s}_i \cdot \vec{n_2})^2 (\vec{s}_i \cdot \vec{n_3})^2$$

with K_1 and K_{2c} (in eV) the intensity coefficients and $\vec{n}_1$, $\vec{n}_2$ and $\vec{n}_3$ defining the three anisotropic directions defined by the command (from *n1x* to *n3z*). For $\vec{n}_1 = (100)$, $\vec{n}_2 = (010)$, and $\vec{n}_3 = (001)$, $K_1 < 0$ defines an iron type anisotropy (easy axis along the (001)-type cube edges), and $K_1 > 0$ defines a nickel type anisotropy (easy axis along the (111)-type cube diagonals). $K_2^c > 0$ also defines easy axis along the (111)-type cube diagonals. See chapter 2 of *(Skomski)* for more details on cubic anisotropies.

In all cases, the choice of (xyz) only imposes the vector directions for the forces. Only the direction of the vector is important; its length is ignored (the entered vectors are normalized).

Those styles can be combined within one single command line.

Restart, fix_modify, output, run start/stop, minimize info:

By default, the energy associated to this fix is not added to the potential energy of the system. The *fix_modify energy* option is supported by this fix to add this magnetic potential energy to the potential energy of the system,

```
fix             1 all precession/spin zeeman 1.0 0.0 0.0 1.0
fix_modify      1 energy yes
```

This fix computes a global scalar which can be accessed by various *output commands*.

No information about this fix is written to *binary restart files*.

16.165.4 Restrictions

The *precession/spin* style is part of the SPIN package. This style is only enabled if LAMMPS was built with this package, and if the atom_style "spin" was declared. See the *Build package* doc page for more info.

16.165.5 Related commands

atom_style spin

Default:

none

(Skomski) Skomski, R. (2008). Simple models of magnetism. Oxford University Press.

16.166 fix press/berendsen command

16.166.1 Syntax

```
fix ID group-ID press/berendsen keyword value ...
```

- ID, group-ID are documented in *fix* command
- press/berendsen = style name of this fix command

```
one or more keyword value pairs may be appended
keyword = iso or aniso or x or y or z or couple or dilate or modulus
  iso or aniso values = Pstart Pstop Pdamp
    Pstart,Pstop = scalar external pressure at start/end of run (pressure␣
↪units)
    Pdamp = pressure damping parameter (time units)
  x or y or z values = Pstart Pstop Pdamp
    Pstart,Pstop = external stress tensor component at start/end of run␣
↪(pressure units)
    Pdamp = stress damping parameter (time units)
  couple = none or xyz or xy or yz or xz
  modulus value = bulk modulus of system (pressure units)
  dilate value = all or partial
```

16.166.2 Examples

```
fix 1 all press/berendsen iso 0.0 0.0 1000.0
fix 2 all press/berendsen aniso 0.0 0.0 1000.0 dilate partial
```

16.166.3 Description

Reset the pressure of the system by using a Berendsen barostat *(Berendsen)*, which rescales the system volume and (optionally) the atoms coordinates within the simulation box every timestep.

Regardless of what atoms are in the fix group, a global pressure is computed for all atoms. Similarly, when the size of the simulation box is changed, all atoms are re-scaled to new positions, unless the keyword *dilate* is specified with a value of *partial*, in which case only the atoms in the fix group are re-scaled. The latter can be useful for leaving the coordinates of atoms in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

Note: Unlike the *fix npt* or *fix nph* commands which perform Nose/Hoover barostatting AND time integration, this fix does NOT perform time integration. It only modifies the box size and atom coordinates to effect barostatting. Thus you must use a separate time integration fix, like *fix nve* or *fix nvt* to actually update the positions and velocities of atoms. This fix can be used in conjunction with thermostatting fixes to control the temperature, such as *fix nvt* or *fix langevin* or *fix temp/berendsen*.

See the *Howto baroostat* doc page for a discussion of different ways to perform barostatting.

The barostat is specified using one or more of the *iso*, *aniso*, *x*, *y*, *z*, and *couple* keywords. These keywords give you the ability to specify the 3 diagonal components of an external stress tensor, and to couple various of these components together so that the dimensions they represent are varied together during a constant-pressure simulation. Unlike the *fix npt* and *fix nph* commands, this fix cannot be used with triclinic (non-orthogonal) simulation boxes to control all 6 components of the general pressure tensor.

The target pressures for each of the 3 diagonal components of the stress tensor can be specified independently via the *x*, *y*, *z*, keywords, which correspond to the 3 simulation box dimensions. For each component, the external pressure or tensor component at each timestep is a ramped value during the run from *Pstart* to *Pstop*. If a target pressure is specified for a component, then the corresponding box dimension will change during a simulation. For example, if the *y* keyword is used, the y-box length will change. A box dimension will not change if that component is not specified, although you have the option to change that dimension via the *fix deform* command.

For all barostat keywords, the *Pdamp* parameter determines the time scale on which pressure is relaxed. For example, a value of 10.0 means to relax the pressure in a timespan of (roughly) 10 time units (tau or fmsec or psec - see the *units* command).

Note: A Berendsen barostat will not work well for arbitrary values of *Pdamp*. If *Pdamp* is too small, the pressure and volume can fluctuate wildly; if it is too large, the pressure will take a very long time to equilibrate. A good choice for many models is a *Pdamp* of around 1000 timesteps. However, note that *Pdamp* is specified in time units, and that timesteps are NOT the same as time units for most *units* settings.

Note: The relaxation time is actually also a function of the bulk modulus of the system (inverse of isothermal compressibility). The bulk modulus has units of pressure and is the amount of pressure that would need to be applied (isotropically) to reduce the volume of the system by a factor of 2 (assuming the bulk modulus was a constant, independent of density, which it's not). The bulk modulus can be set via the keyword *modulus*. The *Pdamp* parameter is effectively multiplied by the bulk modulus, so if the pressure is relaxing faster than expected or desired, increasing the bulk modulus has the same effect as increasing *Pdamp*. The converse is also true. LAMMPS does not attempt to guess a correct value of the bulk modulus; it just uses 10.0 as a default value which gives reasonable relaxation for a Lennard-Jones liquid, but will be way off for other materials and way too small for solids. Thus you should experiment to find appropriate values of *Pdamp* and/or the *modulus* when using this fix.

The *couple* keyword allows two or three of the diagonal components of the pressure tensor to be "coupled" together. The value specified with the keyword determines which are coupled. For example, *xz* means the *Pxx* and *Pzz* components of the stress tensor are coupled. *Xyz* means all 3 diagonal components are coupled. Coupling means two things: the instantaneous stress will be computed as an average of the corresponding diagonal components, and the coupled box dimensions will be changed together in lockstep, meaning coupled dimensions will be dilated or contracted by the same percentage every timestep. The *Pstart*, *Pstop*, *Pdamp* parameters for any coupled dimensions must be identical. *Couple xyz* can be used for a 2d simulation; the *z* dimension is simply ignored.

The *iso* and *aniso* keywords are simply shortcuts that are equivalent to specifying several other keywords together.

The keyword *iso* means couple all 3 diagonal components together when pressure is computed (hydrostatic pressure), and dilate/contract the dimensions together. Using "iso Pstart Pstop Pdamp" is the same as specifying these 4 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
couple xyz
```

The keyword *aniso* means *x*, *y*, and *z* dimensions are controlled independently using the *Pxx*, *Pyy*, and *Pzz* components of the stress tensor as the driving forces, and the specified scalar external pressure. Using "aniso Pstart Pstop Pdamp" is the same as specifying these 4 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
couple none
```

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp group-ID temp
compute fix-ID_press group-ID pressure fix-ID_temp
```

See the *compute temp* and *compute pressure* commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is the same as the fix group.

Note that these are NOT the computes used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the *compute_modify* command or print this temperature or pressure during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify temp* and *press* options are supported by this fix. You can use them to assign a *compute* you have defined to this fix which will be used in its temperature and pressure calculations. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

No global or per-atom quantities are stored by this fix for access by various *output commands*.

This fix can ramp its target pressure over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.166.4 Restrictions

Any dimension being adjusted by this fix must be periodic.

16.166.5 Related commands

fix nve, *fix nph*, *fix npt*, *fix temp/berendsen*, *fix_modify*

16.166.6 Default

The keyword defaults are dilate = all, modulus = 10.0 in units of pressure for whatever *units* are defined.

(Berendsen) Berendsen, Postma, van Gunsteren, DiNola, Haak, J Chem Phys, 81, 3684 (1984).

16.167 fix print command

16.167.1 Syntax

```
fix ID group-ID print N string keyword value ...
```

- ID, group-ID are documented in *fix* command
- print = style name of this fix command

- N = print every N steps; N can be a variable (see below)
- string = text string to print with optional variable names
- zero or more keyword/value pairs may be appended
- keyword = *file* or *append* or *screen* or *title*

```
file value = filename
append value = filename
screen value = yes or no
title value = string
  string =  text to print as 1st line of output file
```

16.167.2 Examples

```
fix extra all print 100 "Coords of marker atom = $x $y $z"
fix extra all print 100 "Coords of marker atom = $x $y $z" file coord.txt
```

16.167.3 Description

Print a text string every N steps during a simulation run. This can be used for diagnostic purposes or as a debugging tool to monitor some quantity during a run. The text string must be a single argument, so it should be enclosed in double quotes if it is more than one word. If it contains variables it must be enclosed in double quotes to insure they are not evaluated when the input script line is read, but will instead be evaluated each time the string is printed.

Instead of a numeric value, N can be specified as an *equal-style variable*, which should be specified as v_name, where name is the variable name. In this case, the variable is evaluated at the beginning of a run to determine the **next** timestep at which the string will be written out. On that timestep, the variable will be evaluated again to determine the next timestep, etc. Thus the variable should return timestep values. See the stagger() and logfreq() and stride() math functions for *equal-style variables*, as examples of useful functions to use in this context. For example, the following commands will print output at timesteps 10,20,30,100,200,300,1000,2000,etc:

```
variable        s equal logfreq(10,3,10)
fix extra all print v_s "Coords of marker atom = $x $y $z"
```

The specified group-ID is ignored by this fix.

See the *variable* command for a description of *equal* style variables which are the most useful ones to use with the fix print command, since they are evaluated afresh each timestep that the fix print line is output. Equal-style variables calculate formulas involving mathematical operations, atom properties, group properties, thermodynamic properties, global values calculated by a *compute* or *fix*, or references to other *variables*.

If the *file* or *append* keyword is used, a filename is specified to which the output generated by this fix will be written. If *file* is used, then the filename is overwritten if it already exists. If *append* is used, then the filename is appended to if it already exists, or created if it does not exist.

If the *screen* keyword is used, output by this fix to the screen and logfile can be turned on or off as desired.

The *title* keyword allow specification of the string that will be printed as the first line of the output file, assuming the *file* keyword was used. By default, the title line is as follows:

```
# Fix print output for fix ID
```

where ID is replaced with the fix-ID.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.167.4 Restrictions

none

16.167.5 Related commands

variable, *print*

16.167.6 Default

The option defaults are no file output, screen = yes, and title string as described above.

16.168 fix propel/self command

16.168.1 Syntax

fix ID group-ID propel/self mode magnitude keyword values ...

- ID, group-ID are documented in *fix* command
- propel/self = style name of this fix command
- mode = velocity or quat
- magnitude = magnitude of the active force
- one or more keyword/value pairs may be appended to args
- keyword = *types*

  types values = one or more atom types

16.168.2 Examples

```
fix active_group all propel/self velocity 1.0
fix constant_velocity all viscous 1.0

fix active_group all propel/self quat 1.0

fix active all propel/self quat 1.0 types 1 2 4
```

16.168.3 Description

Adds a force of a constant magnitude to each atom in the group. The nature in which the force is added depends on the mode.

For *mode* = *velocity*, the active force acts along the velocity vector of each atom. This can be interpreted as a velocity-dependent friction, such as proposed by *(Erdmann)*.

For *mode* = *quat* the force is applied along the axis obtained by rotating the x-axis along the atom's quaternion. In other words, the force is along the x-axis in the atom's body frame. This mode requires all atoms in the group to have a quaternion, so atom_style should either be ellipsoid or body. In combination with Langevin thermostat for translation and rotation in the overdamped regime, the quaternion mode corresponds to the active Brownian particle model introduced by *(Henkes)*, *(Bialke)* and *(Fily)*.

By default, this fix is applied to all atoms in the group. You can override this behavior by specifying the atom types the fix should work on through the *types* keyword.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

This fix is not imposed during minimization.

16.168.4 Restrictions

In quat mode, this fix makes use of per-atom quaternions to take into account the fact that the orientation can rotate and hence the direction of the active force can change. The quat mode of this fix only works with atom_style ellipsoid.

16.168.5 Related commands

fix setforce, *fix addforce*

(Erdmann) U. Erdmann , W. Ebeling, L. Schimansky-Geier, and F. Schweitzer, Eur. Phys. J. B 15, 105-113, 2000.

(Henkes) Henkes, S, Fily, Y., and Marchetti, M. C. Phys. Rev. E, 84, 040301(R), 2011.

(Bialke) J. Bialke, T. Speck, and H Loewen, Phys. Rev. Lett. 108, 168301, 2012.

(Fily) Y. Fily and M.C. Marchetti, Phys. Rev. Lett. 108, 235702, 2012.

Default: types

16.169 fix property/atom command

16.170 fix property/atom/kk command

16.170.1 Syntax

```
fix ID group-ID property/atom vec1 vec2 ... keyword value ...
```

- ID, group-ID are documented in *fix* command
- property/atom = style name of this fix command

- vec1,vec2,... = *mol* or *q* or *rmass* or *i_name* or *d_name*

  ```
  mol = molecule IDs
  q = charge
  rmass = per-atom mass
  i_name = new integer vector referenced by name
  d_name = new floating-point vector referenced by name
  ```

- zero of more keyword/value pairs may be appended
- keyword = *ghost*

  ```
  ghost value = no or yes for whether ghost atom info in communicated
  ```

16.170.2 Examples

```
fix 1 all property/atom mol
fix 1 all property/atom i_myflag1 i_myflag2
fix 1 all property/atom d_sx d_sy d_sz
```

16.170.3 Description

Create one or more additional per-atom vectors to store information about atoms and to use during a simulation. The specified *group-ID* is ignored by this fix.

The atom style used for a simulation defines a set of per-atom properties, as explained on the *atom_style* and *read_data* doc pages. The latter command allows these properties to be defined for each atom in the system when a data file is read. This fix will augment the set of properties with new custom ones. This can be useful in several scenarios.

If the atom style does not define molecule IDs, per-atom charge, or per-atom mass, they can be added using the *mol*, *q* or *rmass* keywords. This can be useful, e.g, to define "molecules" to use as rigid bodies with the *fix rigid* command, or just to carry around an extra flag with the atoms (stored as a molecule ID) that can be used to group atoms without having to use the group command (which is limited to a total of 32 groups including *all*).

Another application would be to use the *rmass* flag in order to have per-atom masses instead of per-type masses, for example this can be useful to study isotope effects with partial isotope substitution. Please *see below* for an example of simulating a mixture of light and heavy water with the TIP4P water potential.

An alternative to using fix *property/atom* in these ways is to use an atom style that does define molecule IDs or charge or per-atom mass (indirectly via diameter and density) or to use a hybrid atom style that combines two or more atom styles to provide the union of all atom properties. However, this has two practical drawbacks: first, it typically necessitates changing the format of the data file, which can be tedious for large systems; and second, it may define additional properties that are not needed such as bond lists, which has some overhead when there are no bonds.

In the future, we may add additional per-atom properties similar to *mol*, *q* or *rmass*, which "turn-on" specific properties defined by some atom styles, so they can be used by atom styles that do not define them.

More generally, the *i_name* and *d_name* vectors allow one or more new custom per-atom properties to be defined. Each name must be unique and can use alphanumeric or underscore characters. These vectors can store whatever values you decide are useful in your simulation. As explained below there are several ways to initialize and access and output these values, both via input script commands and in new code that you add to LAMMPS.

This is effectively a simple way to add per-atom properties to a model without needing to write code for a new *atom style* that defines the properties. Note however that implementing a new atom style allows new atom properties to be more tightly and seamlessly integrated with the rest of the code.

The new atom properties encode values that migrate with atoms to new processors and are written to restart files. If you want the new properties to also be defined for ghost atoms, then use the *ghost* keyword with a value of *yes*. This

will invoke extra communication when ghost atoms are created (at every re-neighboring) to insure the new properties are also defined for the ghost atoms.

Note: If you use this command with the *mol*, *q* or *rmass* vectors, then you most likely want to set *ghost* yes, since these properties are stored with ghost atoms if you use an *atom_style* that defines them, and many LAMMPS operations that use molecule IDs or charge, such as neighbor lists and pair styles, will expect ghost atoms to have these values. LAMMPS will issue a warning it you define those vectors but do not set *ghost* yes.

Note: The properties for ghost atoms are not updated every timestep, but only once every few steps when neighbor lists are re-built. Thus the *ghost* keyword is suitable for static properties, like molecule IDs, but not for dynamic properties that change every step. For the latter, the code you add to LAMMPS to change the properties will also need to communicate their new values to/from ghost atoms, an operation that can be invoked from within a *pair style* or *fix* or *compute* that you write.

Note: If this fix is defined **after** the simulation box is created, a 'run 0' command should be issued to properly initialize the storage created by this fix.

This fix is one of a small number that can be defined in an input script before the simulation box is created or atoms are defined. This is so it can be used with the *read_data* command as described below.

Per-atom properties that are defined by the *atom style* are initialized when atoms are created, e.g. by the *read_data* or *create_atoms* commands. The per-atom properties defined by this fix are not. So you need to initialize them explicitly. This can be done by the *read_data* command, using its *fix* keyword and passing it the fix-ID of this fix.

Thus these commands:

```
fix prop all property/atom mol d_flag
read_data data.txt fix prop NULL Molecules
```

would allow a data file to have a section like this:

```
Molecules

1 4 1.5
2 4 3.0
3 10 1.0
4 10 1.0
5 10 1.0
...
N 763 4.5
```

where N is the number of atoms, and the first field on each line is the atom-ID, followed by a molecule-ID and a floating point value that will be stored in a new property called "flag". Note that the list of per-atom properties can be in any order.

Another way of initializing the new properties is via the *set* command. For example, if you wanted molecules defined for every set of 10 atoms, based on their atom-IDs, these commands could be used:

```
fix prop all property/atom mol
variable cluster atom ((id-1)/10)+1
set atom * mol v_cluster
```

The *atom-style variable* will create values for atoms with IDs 31,32,33,. . . 40 that are 4.0,4.1,4.2,. . . ,4.9. When the *set* commands assigns them to the molecule ID for each atom, they will be truncated to an integer value, so atoms 31-40 will all be assigned a molecule ID of 4.

Note that *atomfile-style variables* can also be used in place of atom-style variables, which means in this case that the molecule IDs could be read-in from a separate file and assigned by the *set* command. This allows you to initialize new per-atom properties in a completely general fashion.

For new atom properties specified as *i_name* or *d_name*, the *compute property/atom* command can access their values. This means that the values can be output via the *dump custom* command, accessed by fixes like *fix ave/atom*, accessed by other computes like *compute reduce*, or used in *atom-style variables*.

For example, these commands will output two new properties to a custom dump file:

```
fix prop all property/atom i_flag1 d_flag2
compute 1 all property/atom i_flag1 d_flag2
dump 1 all custom 100 tmp.dump id x y z c_1[1] c_1[2]
```

If you wish to add new *pair styles*, *fixes*, or *computes* that use the per-atom properties defined by this fix, see the *Modify atom* doc page which has details on how the properties can be accessed from added classes.

Example for using per-atom masses with TIP4P water to study isotope effects. When setting up simulations with the *TIP4P pair styles* for water, you have to provide exactly one atom type each to identify the water oxygen and hydrogen atoms. Since the atom mass is normally tied to the atom type, this makes it impossible to study multiple isotopes in the same simulation. With *fix property/atom rmass* however, the per-type masses are replaced by per-atom masses. Asumming you have a working input deck for regular TIP4P water, where water oxygen is atom type 1 and water hydrogen is atom type 2, the following lines of input script convert this to using per-atom masses:

```
fix Isotopes all property/atom rmass ghost yes
set type 1 mass 15.9994
set type 2 mass 1.008
```

When writing out the system data with the *write_data* command, there will be a new section named with the fix-ID (i.e. *Isotopes* in this case). Alternatively, you can take an existing data file and just add this *Isotopes* section with one line per atom containing atom-ID and mass. Either way, the extended data file can be read back with:

```
fix Isotopes all property/atom rmass ghost yes
read_data tip4p-isotopes.data fix Isotopes NULL Isotopes
```

Please note that the first *Isotopes* refers to the fix-ID and the second to the name of the section. The following input script code will now change the first 100 water molecules in this example to heavy water:

```
group hwat id 2:300:3
group hwat id 3:300:3
set group hwat mass 2.0141018
```

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the per-atom values it stores to *binary restart files*, so that the values can be restored when a simulation is restarted. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.170.4 Restrictions

none

16.170.5 Related commands

read_data, *set*, *compute property/atom*

16.170.6 Default

The default keyword values are ghost = no.

16.171 fix python/invoke command

16.171.1 Syntax

```
fix ID group-ID python/invoke N callback function_name
```

- ID, group-ID are ignored by this fix
- python/invoke = style name of this fix command
- N = execute every N steps
- callback = *post_force* or *end_of_step*

  post_force = callback after force computations on atoms every N time steps
  end_of_step = callback after every N time steps

16.171.2 Examples

```
python post_force_callback here """
from lammps import lammps

def post_force_callback(lammps_ptr, vflag):
    lmp = lammps(ptr=lammps_ptr)
    # access LAMMPS state using Python interface
"""

python end_of_step_callback here """
def end_of_step_callback(lammps_ptr):
    lmp = lammps(ptr=lammps_ptr)
    # access LAMMPS state using Python interface
"""

fix pf  all python/invoke 50 post_force post_force_callback
fix eos all python/invoke 50 end_of_step end_of_step_callback
```

16.171.3 Description

This fix allows you to call a Python function during a simulation run. The callback is either executed after forces have been applied to atoms or at the end of every N time steps.

Callback functions must be declared in the global scope of the active Python interpreter. This can either be done by defining it inline using the python command or by importing functions from other Python modules. If LAMMPS is driven using the library interface from Python, functions defined in the driving Python interpreter can also be executed.

Each callback is given a pointer object as first argument. This can be used to initialize an instance of the lammps Python interface, which gives access to the LAMMPS state from Python.

Warning: While you can access the state of LAMMPS via library functions from these callbacks, trying to execute input script commands will in the best case not work or in the worst case result in undefined behavior.

16.171.4 Restrictions

This fix is part of the PYTHON package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Building LAMMPS with the PYTHON package will link LAMMPS with the Python library on your system. Settings to enable this are in the lib/python/Makefile.lammps file. See the lib/python/README file for information on those settings.

16.171.5 Related commands

python command

16.172 fix python/move command

16.172.1 Syntax

```
fix python/move pymodule.CLASS
```

pymodule.CLASS = use class **CLASS** in module/file **pymodule** to compute how to move atoms

16.172.2 Examples

```
fix  1 all python/move py_nve.NVE
fix  1 all python/move py_nve.NVE_OPT
```

16.172.3 Description

The *python/move* fix style provides a way to define ways how particles are moved during an MD run from python script code, that is loaded from a file into LAMMPS and executed at the various steps where other fixes can be executed. This python script must contain specific python class definitions.

This allows to implement complex position updates and also modified time integration methods. Due to python being an interpreted language, however, the performance of this fix can be moderately to significantly slower than the corresponding C++ code. For specific cases, this performance penalty can be limited through effective use of NumPy.

The python module file has to start with the following code:

```
from __future__ import print_function
import lammps
import ctypes
import traceback
import numpy as np
#
class LAMMPSFix(object):
    def __init__(self, ptr, group_name="all"):
        self.lmp = lammps.lammps(ptr=ptr)
        self.group_name = group_name
#
class LAMMPSFixMove(LAMMPSFix):
    def __init__(self, ptr, group_name="all"):
        super(LAMMPSFixMove, self).__init__(ptr, group_name)
#
    def init(self):
        pass
#
    def initial_integrate(self, vflag):
        pass
```

```
#
    def final_integrate(self):
        pass
#
    def initial_integrate_respa(self, vflag, ilevel, iloop):
        pass
#
    def final_integrate_respa(self, ilevel, iloop):
        pass
#
    def reset_dt(self):
        pass
```

Any classes implementing new atom motion functionality have to be derived from the **LAMMPSFixMove** class, overriding the available methods as needed.

Examples for how to do this are in the *examples/python* folder.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.172.4 Restrictions

This pair style is part of the PYTHON package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.172.5 Related commands

fix nve, *fix python/invoke*

Default: none

16.173 fix qbmsst command

16.173.1 Syntax

```
fix ID group-ID qbmsst dir shockvel keyword value ...
```

- ID, group-ID are documented in *fix* command
- qbmsst = style name of this fix
- dir = *x* or *y* or *z*
- shockvel = shock velocity (strictly positive, velocity units)
- zero or more keyword/value pairs may be appended
- keyword = *q* or *mu* or *p0* or *v0* or *e0* or *tscale* or *damp* or *seed*or *f_max* or *N_f* or *eta* or *beta* or *T_init*

```
q value = cell mass-like parameter (mass^2/distance^4 units)
mu value = artificial viscosity (mass/distance/time units)
p0 value = initial pressure in the shock equations (pressure units)
v0 value = initial simulation cell volume in the shock equations␣
↪(distance^3 units)
e0 value = initial total energy (energy units)
tscale value = reduction in initial temperature (unitless fraction␣
↪between 0.0 and 1.0)
damp value = damping parameter (time units) inverse of friction gamma
seed value = random number seed (positive integer)
f_max value = upper cutoff frequency of the vibration spectrum (1/time␣
↪units)
N_f value = number of frequency bins (positive integer)
eta value = coupling constant between the shock system and the quantum␣
↪thermal bath (positive unitless)
beta value = the quantum temperature is updated every beta time steps␣
↪(positive integer)
T_init value = quantum temperature for the initial state (temperature␣
↪units)
```

16.173.2 Examples

```
# (liquid methane modeled with the REAX force field, real units)
fix 1 all qbmsst z 0.122 q 25 mu 0.9 tscale 0.01 damp 200 seed 35082 f_max 0.3 N_f␣
↪100 eta 1 beta 400 T_init 110
# (quartz modeled with the BKS force field, metal units)
fix 2 all qbmsst z 72 q 40 tscale 0.05 damp 1 seed 47508 f_max 120.0 N_f 100 eta 1.0␣
↪beta 500 T_init 300
```

Two example input scripts are given, including shocked α-quartz and shocked liquid methane. The input script first equilibrates an initial state with the quantum thermal bath at the target temperature and then applies *fix qbmsst* to simulate shock compression with quantum nuclear correction. The following two figures plot relevant quantities for shocked α-quartz.

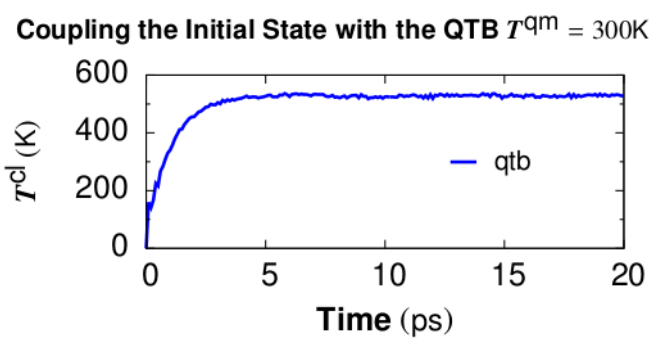


Figure 1. Classical temperature $T_{cl} = \sum \frac{m_i v_i^2}{3Nk_B}$ vs. time for coupling the α-quartz initial state with the quantum thermal bath at target quantum temperature $T^{qm} = 300K$. The NpH ensemble is used for time integration while QTB provides the colored random force. T^{cl} converges at the timescale of *damp* which is set to be 1 ps.

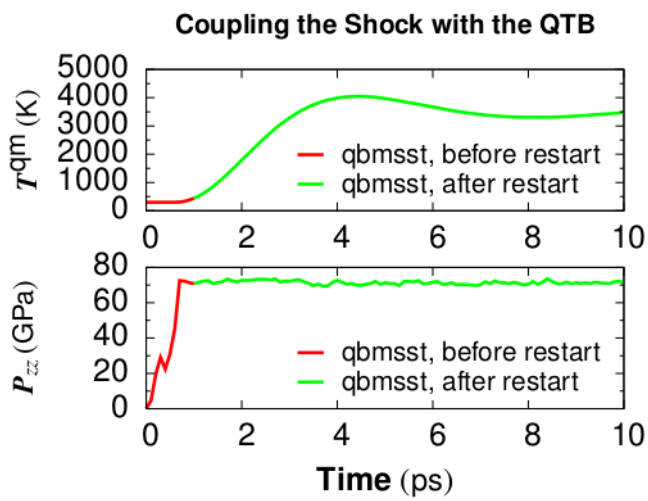


Figure 2. Quantum temperature and pressure vs. time for simulating shocked α-quartz with *fix qbmsst*. The shock propagates along the z direction. Restart of the *fix qbmsst* command is demonstrated in the example input script. Thermodynamic quantities stay continuous before and after the restart.

16.173.3 Description

This command performs the Quantum-Bath coupled Multi-Scale Shock Technique (QBMSST) integration. See *(Qi)* for a detailed description of this method. QBMSST provides description of the thermodynamics and kinetics of shock processes while incorporating quantum nuclear effects. The *shockvel* setting determines the steady shock velocity that will be simulated along direction *dir*.

Quantum nuclear effects *(fix qtb)* can be crucial especially when the temperature of the initial state is below the classical limit or there is a great change in the zero point energies between the initial and final states. Theoretical post processing quantum corrections of shock compressed water and methane have been reported as much as 30% of the temperatures *(Goldman)*. A self-consistent method that couples the shock to a quantum thermal bath described by a colored noise Langevin thermostat has been developed by Qi et al *(Qi)* and applied to shocked methane. The onset of chemistry is reported to be at a pressure on the shock Hugoniot that is 40% lower than observed with classical molecular dynamics.

It is highly recommended that the system be already in an equilibrium state with a quantum thermal bath at temperature of *T_init*. The fix command *fix qtb* at constant temperature *T_init* could be used before applying this command to introduce self-consistent quantum nuclear effects into the initial state.

The parameters *q*, *mu*, *e0*, *p0*, *v0* and *tscale* are described in the command *fix msst*. The values of *e0*, *p0*, or *v0* will be calculated on the first step if not specified. The parameter of *damp*, *f_max*, and *N_f* are described in the command *fix qtb*.

The *fix qbmsst* command couples the shock system to a quantum thermal bath with a rate that is proportional to the change of the total energy of the shock system, $E^{tot} - E_0^{tot}$. Here E^{etot} consists of both the system energy and a thermal term, see *(Qi)*, and $E_0^{tot} = e0$ is the initial total energy.

The *eta* (η) parameter is a unitless coupling constant between the shock system and the quantum thermal bath. A small η value cannot adjust the quantum temperature fast enough during the temperature ramping period of shock compression while large η leads to big temperature oscillation. A value of η between 0.3 and 1 is usually appropriate for simulating most systems under shock compression. We observe that different values of η lead to almost the same final thermodynamic state behind the shock, as expected.

The quantum temperature is updated every *beta* (β) steps with an integration time interval β times longer than the simulation time step. In that case, E^{tot} is taken as its average over the past β steps. The temperature of the quantum

thermal bath T^{qm} changes dynamically according to the following equation where Δ_t is the MD time step and γ is the friction constant which is equal to the inverse of the *damp* parameter.

$$\frac{dT^{qm}}{dt} = \gamma\eta \sum_{l=1}^{\beta} \frac{E^{tot}(t - l\Delta t) - E_0^{tot}}{3\beta N k_B}$$

The parameter *T_init* is the initial temperature of the quantum thermal bath and the system before shock loading.

For all pressure styles, the simulation box stays orthorhombic in shape. Parrinello-Rahman boundary conditions (tilted box) are supported by LAMMPS, but are not implemented for QBMSST.

Restart, fix_modify, output, run start/stop, minimize info:

Because the state of the random number generator is not written to *binary restart files*, this fix cannot be restarted "exactly" in an uninterrupted fashion. However, in a statistical sense, a restarted simulation should produce similar behaviors of the system as if it is not interrupted. To achieve such a restart, one should write explicitly the same value for *q*, *mu*, *damp*, *f_max*, *N_f*, *eta*, and *beta* and set *tscale* = 0 if the system is compressed during the first run.

The progress of the QBMSST can be monitored by printing the global scalar and global vector quantities computed by the fix. The global vector contains five values in this order:

[*dhugoniot*, *drayleigh*, *lagrangian_speed*, *lagrangian_position*, *quantum_temperature*]

1. *dhugoniot* is the departure from the Hugoniot (temperature units).
2. *drayleigh* is the departure from the Rayleigh line (pressure units).
3. *lagrangian_speed* is the laboratory-frame Lagrangian speed (particle velocity) of the computational cell (velocity units).
4. *lagrangian_position* is the computational cell position in the reference frame moving at the shock speed. This is the distance of the computational cell behind the shock front.
5. *quantum_temperature* is the temperature of the quantum thermal bath T^{qm}.

To print these quantities to the log file with descriptive column headers, the following LAMMPS commands are suggested. Here the *fix_modify* energy command is also enabled to allow the thermo keyword *etotal* to print the quantity E^{tot}. See also the *thermo_style* command.

```
fix             fix_id all msst z
fix_modify      fix_id energy yes
variable        dhug    equal f_fix_id[1]
variable        dray    equal f_fix_id[2]
variable        lgr_vel equal f_fix_id[3]
variable        lgr_pos equal f_fix_id[4]
variable        T_qm    equal f_fix_id[5]
thermo_style    custom  step temp ke pe lz pzz etotal v_dhug v_dray v_lgr_vel v_lgr_
↪pos v_T_qm f_fix_id
```

The global scalar under the entry f_fix_id is the quantity of thermo energy as an extra part of E^{tot}. This global scalar and the vector of 5 quantities can be accessed by various *output commands*. It is worth noting that the temp keyword under the *thermo_style* command print the instantaneous classical temperature T^{cl} as described in the command *fix qtb*.

16.173.4 Restrictions

This fix style is part of the USER-QTB package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

All cell dimensions must be periodic. This fix can not be used with a triclinic cell. The QBMSST fix has been tested only for the group-ID all.

16.173.5 Related commands

fix qtb, *fix msst*

16.173.6 Default

The keyword defaults are q = 10, mu = 0, tscale = 0.01, damp = 1, seed = 880302, f_max = 200.0, N_f = 100, eta = 1.0, beta = 100, and T_init=300.0. e0, p0, and v0 are calculated on the first step.

(Goldman) Goldman, Reed and Fried, J. Chem. Phys. 131, 204103 (2009)

(Qi) Qi and Reed, J. Phys. Chem. A 116, 10451 (2012).

16.174 fix qeq/point command

16.175 fix qeq/shielded command

16.176 fix qeq/slater command

16.177 fix qeq/dynamic command

16.178 fix qeq/fire command

16.178.1 Syntax

```
fix ID group-ID style Nevery cutoff tolerance maxiter qfile keyword ...
```

- ID, group-ID are documented in *fix* command
- style = *qeq/point* or *qeq/shielded* or *qeq/slater* or *qeq/dynamic* or *qeq/fire*
- Nevery = perform charge equilibration every this many steps
- cutoff = global cutoff for charge-charge interactions (distance unit)
- tolerance = precision to which charges will be equilibrated

- maxiter = maximum iterations to perform charge equilibration
- qfile = a filename with QEq parameters or *coul/streitz* or *reax/c*
- zero or more keyword/value pairs may be appended
- keyword = *alpha* or *qdamp* or *qstep*

```
alpha value = Slater type orbital exponent (qeq/slater only)
qdamp value = damping factor for damped dynamics charge solver (qeq/
↪dynamic and qeq/fire only)
qstep value = time step size for damped dynamics charge solver (qeq/
↪dynamic and qeq/fire only)
```

16.178.2 Examples

```
fix 1 all qeq/point 1 10 1.0e-6 200 param.qeq1
fix 1 qeq qeq/shielded 1 8 1.0e-6 100 param.qeq2
fix 1 all qeq/slater 5 10 1.0e-6 100 params alpha 0.2
fix 1 qeq qeq/dynamic 1 12 1.0e-3 100 my_qeq
fix 1 all qeq/fire 1 10 1.0e-3 100 my_qeq qdamp 0.2 qstep 0.1
```

16.178.3 Description

Perform the charge equilibration (QEq) method as described in *(Rappe and Goddard)* and formulated in *(Nakano)* (also known as the matrix inversion method) and in *(Rick and Stuart)* (also known as the extended Lagrangian method) based on the electronegativity equilization principle.

These fixes can be used with any *pair style* in LAMMPS, so long as per-atom charges are defined. The most typical use-case is in conjunction with a *pair style* that performs charge equilibration periodically (e.g. every timestep), such as the ReaxFF or Streitz-Mintmire potential. But these fixes can also be used with potentials that normally assume per-atom charges are fixed, e.g. a *Buckingham* or *LJ/Coulombic* potential.

Because the charge equilibration calculation is effectively independent of the pair style, these fixes can also be used to perform a one-time assignment of charges to atoms. For example, you could define the QEq fix, perform a zero-timestep run via the *run* command without any pair style defined which would set per-atom charges (based on the current atom configuration), then remove the fix via the *unfix* command before performing further dynamics.

Note: Computing and using charge values different from published values defined for a fixed-charge potential like Buckingham or CHARMM or AMBER, can have a strong effect on energies and forces, and produces a different model than the published versions.

Note: The *fix qeq/comb* command must still be used to perform charge equilibration with the *COMB potential*. The *fix qeq/reax* command can be used to perform charge equilibration with the *ReaxFF force field*, although fix qeq/shielded yields the same results as fix qeq/reax if *Nevery*, *cutoff*, and *tolerance* are the same. Eventually the fix qeq/reax command will be deprecated.

The QEq method minimizes the electrostatic energy of the system (or equalizes the derivative of energy with respect to charge of all the atoms) by adjusting the partial charge on individual atoms based on interactions with their neighbors within *cutoff*. It requires a few parameters, in *metal* units, for each atom type which provided in a file specified by *qfile*. The file has the following format

```
1 chi eta gamma zeta qcore
2 chi eta gamma zeta qcore
...
Ntype chi eta gamma zeta qcore
```

There have to be parameters given for every atom type. Wildcard entries are possible using the same syntax as elsewhere in LAMMPS (i.e., n*m, n*, *m, *). Later entries will overwrite previous ones. Empty lines or any text following the pound sign (#) are ignored. Each line starts with the atom type followed by five parameters. Only a subset of the parameters is used by each QEq style as described below, thus the others can be set to 0.0 if desired, but all five entries per line are required.

- *chi* = electronegativity in energy units
- *eta* = self-Coulomb potential in energy units
- *gamma* = shielded Coulomb constant defined by *ReaxFF force field* in distance units
- *zeta* = Slater type orbital exponent defined by the *Streitz-Mintmire* potential in reverse distance units
- *qcore* = charge of the nucleus defined by the *Streitz-Mintmire potential* potential in charge units

The *qeq/point* style describes partial charges on atoms as point charges. Interaction between a pair of charged particles is 1/r, which is the simplest description of the interaction between charges. Only the *chi* and *eta* parameters from the *qfile* file are used. Note that Coulomb catastrophe can occur if repulsion between the pair of charged particles is too weak. This style solves partial charges on atoms via the matrix inversion method. A tolerance of 1.0e-6 is usually a good number.

The *qeq/shielded* style describes partial charges on atoms also as point charges, but uses a shielded Coulomb potential to describe the interaction between a pair of charged particles. Interaction through the shielded Coulomb is given by equation (13) of the *ReaxFF force field* paper. The shielding accounts for charge overlap between charged particles at small separation. This style is the same as *fix qeq/reax*, and can be used with *pair_style reax/c*. Only the *chi*, *eta*, and *gamma* parameters from the *qfile* file are used. When using the string *reax/c* as filename, these parameters are extracted directly from an active *reax/c* pair style. This style solves partial charges on atoms via the matrix inversion method. A tolerance of 1.0e-6 is usually a good number.

The *qeq/slater* style describes partial charges on atoms as spherical charge densities centered around atoms via the Slater 1*s* orbital, so that the interaction between a pair of charged particles is the product of two Slater 1*s* orbitals. The expression for the Slater 1*s* orbital is given under equation (6) of the *Streitz-Mintmire* paper. Only the *chi*, *eta*, *zeta*, and *qcore* parameters from the *qfile* file are used. When using the string *coul/streitz* as filename, these parameters are extracted directly from an active *coul/streitz* pair style. This style solves partial charges on atoms via the matrix inversion method. A tolerance of 1.0e-6 is usually a good number. Keyword *alpha* can be used to change the Slater type orbital exponent.

The *qeq/dynamic* style describes partial charges on atoms as point charges that interact through 1/r, but the extended Lagrangian method is used to solve partial charges on atoms. Only the *chi* and *eta* parameters from the *qfile* file are used. Note that Coulomb catastrophe can occur if repulsion between the pair of charged particles is too weak. A tolerance of 1.0e-3 is usually a good number. Keyword *qdamp* can be used to change the damping factor, while keyword *qstep* can be used to change the time step size.

The **qeq/fire** style describes the same charge model and charge solver as the *qeq/dynamic* style, but employs a FIRE minimization algorithm to solve for equilibrium charges. Keyword *qdamp* can be used to change the damping factor, while keyword *qstep* can be used to change the time step size.

Note that *qeq/point*, *qeq/shielded*, and *qeq/slater* describe different charge models, whereas the matrix inversion method and the extended Lagrangian method (*qeq/dynamic* and *qeq/fire*) are different solvers.

Note that *qeq/point*, *qeq/dynamic* and *qeq/fire* styles all describe charges as point charges that interact through 1/r relationship, but solve partial charges on atoms using different solvers. These three styles should yield comparable results if the QEq parameters and *Nevery*, *cutoff*, and *tolerance* are the same. Style *qeq/point* is typically faster, *qeq/dynamic* scales better on larger sizes, and *qeq/fire* is faster than *qeq/dynamic*.

Note: To avoid the evaluation of the derivative of charge with respect to position, which is typically ill-defined, the system should have a zero net charge.

Note: Developing QEq parameters (chi, eta, gamma, zeta, and qcore) is non-trivial. Charges on atoms are not guaranteed to equilibrate with arbitrary choices of these parameters. We do not develop these QEq parameters. See the examples/qeq directory for some examples.

Restart, fix_modify, output, run start/stop, minimize info:

No information about these fixes is written to *binary restart files*. No global scalar or vector or per-atom quantities are stored by these fixes for access by various *output commands*. No parameter of these fixes can be used with the *start/stop* keywords of the *run* command.

Thexe fixes are invoked during *energy minimization*.

16.178.4 Restrictions

These fixes are part of the QEQ package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.178.5 Related commands

fix qeq/reax, *fix qeq/comb*

Default: none

(Rappe and Goddard) A. K. Rappe and W. A. Goddard III, J Physical Chemistry, 95, 3358-3363 (1991).

(Nakano) A. Nakano, Computer Physics Communications, 104, 59-69 (1997).

(Rick and Stuart) S. W. Rick, S. J. Stuart, B. J. Berne, J Chemical Physics 101, 16141 (1994).

(Streitz-Mintmire) F. H. Streitz, J. W. Mintmire, Physical Review B, 50, 16, 11996 (1994)

(ReaxFF) A. C. T. van Duin, S. Dasgupta, F. Lorant, W. A. Goddard III, J Physical Chemistry, 105, 9396-9049 (2001)

(QEq/Fire) T.-R. Shan, A. P. Thompson, S. J. Plimpton, in preparation

16.179 fix qeq/comb command

16.180 fix qeq/comb/omp command

16.180.1 Syntax

```
fix ID group-ID qeq/comb Nevery precision keyword value ...
```

- ID, group-ID are documented in *fix* command
- qeq/comb = style name of this fix command

- Nevery = perform charge equilibration every this many steps
- precision = convergence criterion for charge equilibration
- zero or more keyword/value pairs may be appended
- keyword = *file*

```
file value = filename
  filename = name of file to write QEQ equilibration info to
```

16.180.2 Examples

```
fix 1 surface qeq/comb 10 0.0001
```

16.180.3 Description

Perform charge equilibration (QeQ) in conjunction with the COMB (Charge-Optimized Many-Body) potential as described in *(COMB_1)* and *(COMB_2)*. It performs the charge equilibration portion of the calculation using the so-called QEq method, whereby the charge on each atom is adjusted to minimize the energy of the system. This fix can only be used with the COMB potential; see the *fix qeq/reax* command for a QeQ calculation that can be used with any potential.

Only charges on the atoms in the specified group are equilibrated. The fix relies on the pair style (COMB in this case) to calculate the per-atom electronegativity (effective force on the charges). An electronegativity equalization calculation (or QEq) is performed in an iterative fashion, which in parallel requires communication at each iteration for processors to exchange charge information about nearby atoms with each other. See *Rappe_and_Goddard* and *Rick_and_Stuart* for details.

During a run, charge equilibration is performed every *Nevery* time steps. Charge equilibration is also always enforced on the first step of each run. The *precision* argument controls the tolerance for the difference in electronegativity for all atoms during charge equilibration. *Precision* is a trade-off between the cost of performing charge equilibration (more iterations) and accuracy.

If the *file* keyword is used, then information about each equilibration calculation is written to the specified file.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix is performing charge equilibration. Default is the outermost level.

This fix produces a per-atom vector which can be accessed by various *output commands*. The vector stores the gradient of the charge on each atom. The per-atom values be accessed on any timestep.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

This fix can be invoked during *energy minimization*.

16.180.4 Restrictions

This fix command currently only supports *pair style *comb**.

16.180.5 Related commands

pair_style comb

16.180.6 Default

No file output is performed.

(COMB_1) J. Yu, S. B. Sinnott, S. R. Phillpot, Phys Rev B, 75, 085311 (2007),

(COMB_2) T.-R. Shan, B. D. Devine, T. W. Kemper, S. B. Sinnott, S. R. Phillpot, Phys Rev B, 81, 125328 (2010).

(Rappe_and_Goddard) A. K. Rappe, W. A. Goddard, J Phys Chem 95, 3358 (1991).

(Rick_and_Stuart) S. W. Rick, S. J. Stuart, B. J. Berne, J Chem Phys 101, 16141 (1994).

16.181 fix qeq/reax command

16.182 fix qeq/reax/kk command

16.183 fix qeq/reax/omp command

16.183.1 Syntax

```
fix ID group-ID qeq/reax Nevery cutlo cuthi tolerance params args
```

- ID, group-ID are documented in *fix* command
- qeq/reax = style name of this fix command
- Nevery = perform QEq every this many steps
- cutlo,cuthi = lo and hi cutoff for Taper radius
- tolerance = precision to which charges will be equilibrated
- params = reax/c or a filename
- args = *dual* (optional)

16.183.2 Examples

```
fix 1 all qeq/reax 1 0.0 10.0 1.0e-6 reax/c
fix 1 all qeq/reax 1 0.0 10.0 1.0e-6 param.qeq
```

16.183.3 Description

Perform the charge equilibration (QEq) method as described in *(Rappe and Goddard)* and formulated in *(Nakano)*. It is typically used in conjunction with the ReaxFF force field model as implemented in the *pair_style reax/c* command, but it can be used with any potential in LAMMPS, so long as it defines and uses charges on each atom. The *fix qeq/comb* command should be used to perform charge equilibration with the *COMB potential*. For more technical details about the charge equilibration performed by fix qeq/reax, see the *(Aktulga)* paper.

The QEq method minimizes the electrostatic energy of the system by adjusting the partial charge on individual atoms based on interactions with their neighbors. It requires some parameters for each atom type. If the *params* setting above is the word "reax/c", then these are extracted from the *pair_style reax/c* command and the ReaxFF force field file it reads in. If a file name is specified for *params*, then the parameters are taken from the specified file and the file must contain one line for each atom type. The latter form must be used when performing QeQ with a non-ReaxFF potential. Each line should be formatted as follows:

```
itype chi eta gamma
```

where *itype* is the atom type from 1 to Ntypes, *chi* denotes the electronegativity in eV, *eta* denotes the self-Coulomb potential in eV, and *gamma* denotes the valence orbital exponent. Note that these 3 quantities are also in the ReaxFF potential file, except that eta is defined here as twice the eta value in the ReaxFF file. Note that unlike the rest of LAMMPS, the units of this fix are hard-coded to be A, eV, and electronic charge.

The optional *dual* keyword allows to perform the optimization of the S and T matrices in parallel. This is only supported for the *qeq/reax/omp* style. Otherwise they are processed separately.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. No global scalar or vector or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

This fix is invoked during *energy minimization*.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

16.183.4 Restrictions

This fix is part of the USER-REAXC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix does not correctly handle interactions involving multiple periodic images of the same atom. Hence, it should not be used for periodic cell dimensions less than 10 angstroms.

16.183.5 Related commands

pair_style reax/c

Default: none

(Rappe) Rappe and Goddard III, Journal of Physical Chemistry, 95, 3358-3363 (1991).

(Nakano) Nakano, Computer Physics Communications, 104, 59-69 (1997).

(Aktulga) Aktulga, Fogarty, Pandit, Grama, Parallel Computing, 38, 245-259 (2012).

16.184 fix qmmm command

16.184.1 Syntax

```
fix ID group-ID qmmm
```

- ID, group-ID are documented in *fix* command
- qmmm = style name of this fix command

16.184.2 Examples

fix 1 qmol qmmm

16.184.3 Description

This fix provides functionality to enable a quantum mechanics/molecular mechanics (QM/MM) coupling of LAMMPS to a quantum mechanical code. The current implementation only supports an ONIOM style mechanical coupling to the Quantum ESPRESSO plane wave DFT package. Electrostatic coupling is in preparation and the interface has been written in a manner that coupling to other QM codes should be possible without changes to LAMMPS itself.

The interface code for this is in the lib/qmmm directory of the LAMMPS distribution and is being made available at this early stage of development in order to encourage contributions for interfaces to other QM codes. This will allow the LAMMPS side of the implementation to be adapted if necessary before being finalized.

Details about how to use this fix are currently documented in the description of the QM/MM interface code itself in lib/qmmm/README.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global scalar or vector or per-atom quantities are stored by this fix for access by various *output commands*. No

parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.184.4 Restrictions

This fix is part of the USER-QMMM package. It is only enabled if LAMMPS was built with that package. It also requires building a library provided with LAMMPS. See the *Build package* doc page for more info.

The fix is only functional when LAMMPS is built as a library and linked with a compatible QM program and a QM/MM front end into a QM/MM executable. See the lib/qmmm/README file for details.

Related commands: none

Default: none

16.185 fix qtb command

16.185.1 Syntax

```
fix ID group-ID qtb keyword value ...
```

- ID, group-ID are documented in *fix* command
- qtb = style name of this fix
- zero or more keyword/value pairs may be appended
- keyword = *temp* or *damp* or *seed* or *f_max* or *N_f*

```
temp value = target quantum temperature (temperature units)
damp value = damping parameter (time units) inverse of friction gamma
seed value = random number seed (positive integer)
f_max value = upper cutoff frequency of the vibration spectrum (1/time␣
↪units)
N_f value = number of frequency bins (positive integer)
```

16.185.2 Examples

```
# (liquid methane modeled with the REAX force field, real units)
fix 1 all nve
fix 1 all qtb temp 110 damp 200 seed 35082 f_max 0.3 N_f 100
# (quartz modeled with the BKS force field, metal units)
fix 2 all nph iso 1.01325 1.01325 1
fix 2 all qtb temp 300 damp 1 seed 47508 f_max 120.0 N_f 100
```

16.185.3 Description

This command performs the quantum thermal bath scheme proposed by *(Dammak)* to include self-consistent quantum nuclear effects, when used in conjunction with the *fix nve* or *fix nph* commands.

Classical molecular dynamics simulation does not include any quantum nuclear effect. Quantum treatment of the vibrational modes will introduce zero point energy into the system, alter the energy power spectrum and bias the heat capacity from the classical limit. Missing all the quantum nuclear effects, classical MD cannot model systems at temperatures lower than their classical limits. This effect is especially important for materials with a large population of hydrogen atoms and thus higher classical limits.

The equation of motion implemented by this command follows a Langevin form:

$$m_i a_i = f_i + R_i - m_i \gamma v_i$$

Here $m_i, a_i, f_i, R_i, \gamma,$ andv_i represent in this order mass, acceleration, force exerted by all other atoms, random force, frictional coefficient (the inverse of damping parameter damp), and velocity. The random force R_i is "colored" so that any vibrational mode with frequency ω will have a temperature-sensitive energy $\theta(\omega, T)$ which resembles the energy expectation for a quantum harmonic oscillator with the same natural frequency:

$$\theta(\omega T) = \frac{\hbar}{2} + \hbar\omega \left[\exp(\frac{\hbar\omega}{k_B T}) - 1\right]^{-1}$$

To efficiently generate the random forces, we employ the method of *(Barrat)*, that circumvents the need to generate all random forces for all times before the simulation. The memory requirement of this approach is less demanding and independent of the simulation duration. Since the total random force R_{tot} does not necessarily vanish for a finite number of atoms, R_i is replaced by $R_i - \frac{R_{tot}}{N_{tot}}$ to avoid collective motion of the system.

The *temp* parameter sets the target quantum temperature. LAMMPS will still have an output temperature in its thermo style. That is the instantaneous classical temperature T^{cl} derived from the atom velocities at thermal equilibrium. A non-zero T^{cl} will be present even when the quantum temperature approaches zero. This is associated with zero-point energy at low temperatures.

$$T^{cl} = \sum \frac{m_i v_i^2}{3Nk_B}$$

The *damp* parameter is specified in time units, and it equals the inverse of the frictional coefficient γ. γ should be as small as possible but slightly larger than the timescale of anharmonic coupling in the system which is about 10 ps to 100 ps. When γ is too large, it gives an energy spectrum that differs from the desired Bose-Einstein spectrum. When γ is too small, the quantum thermal bath coupling to the system will be less significant than anharmonic effects, reducing to a classical limit. We find that setting γ between 5 THz and 1 THz could be appropriate depending on the system.

The random number *seed* is a positive integer used to initiate a Marsaglia random number generator. Each processor uses the input seed to generate its own unique seed and its own stream of random numbers. Thus the dynamics of the system will not be identical on two runs on different numbers of processors.

The *f_max* parameter truncate the noise frequency domain so that vibrational modes with frequencies higher than *f_max* will not be modulated. If we denote Δt as the time interval for the MD integration, *f_max* is always reset by the code to make $\alpha = (int)(2\,f_max\,\Delta t)^{-1}$ a positive integer and print out relative information. An appropriate value for the cutoff frequency *f_max* would be around 2~3 f_D, where f_D is the Debye frequency.

The *N_f* parameter is the frequency grid size, the number of points from 0 to *f_max* in the frequency domain that will be sampled. 3*2*N_f* per-atom random numbers are required in the random force generation and there could be as many atoms as in the whole simulation that can migrate into every individual processor. A larger *N_f* provides a more accurate sampling of the spectrum while consumes more memory. With fixed *f_max* and γ, *N_f* should be big enough to converge the classical temperature T^{cl} as a function of target quantum bath temperature. Memory usage per processor could be from 10 to 100 Mbytes.

Note: Unlike the *fix nvt* command which performs Nose/Hoover thermostatting AND time integration, this fix does NOT perform time integration. It only modifies forces to a colored thermostat. Thus you must use a separate time integration fix, like *fix nve* or *fix nph* to actually update the velocities and positions of atoms (as shown in the examples). Likewise, this fix should not normally be used with other fixes or commands that also specify system temperatures , e.g. *fix nvt* and *fix temp/rescale*.

Restart, fix_modify, output, run start/stop, minimizie info:

No information about this fix is written to *binary restart files*. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix. However, in a statistical sense, a restarted simulation should produce similar behaviors of the system.

This fix is not invoked during *energy minimization*.

16.185.4 Restrictions

This fix style is part of the USER-QTB package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.185.5 Related commands

fix nve, *fix nph*, *fix langevin*, *fix qbmsst*

16.185.6 Default

The keyword defaults are temp = 300, damp = 1, seed = 880302, f_max=200.0 and N_f = 100.

(Dammak) Dammak, Chalopin, Laroche, Hayoun, and Greffet, Phys Rev Lett, 103, 190601 (2009).

(Barrat) Barrat and Rodney, J. Stat. Phys, 144, 679 (2011).

16.186 fix reax/c/bonds command

16.187 fix reax/c/bonds/kk command

16.187.1 Syntax

```
fix ID group-ID reaxc/bonds Nevery filename
```

- ID, group-ID are documented in *fix* command

- reax/bonds = style name of this fix command
- Nevery = output interval in timesteps
- filename = name of output file

16.187.2 Examples

```
fix 1 all reax/c/bonds 100 bonds.reaxc
```

16.187.3 Description

Write out the bond information computed by the ReaxFF potential specified by *pair_style reax/c* in the exact same format as the original stand-alone ReaxFF code of Adri van Duin. The bond information is written to *filename* on timesteps that are multiples of *Nevery*, including timestep 0. For time-averaged chemical species analysis, please see the *fix reaxc/c/species* command.

The specified group-ID is ignored by this fix.

The format of the output file should be reasonably self-explanatory. The meaning of the column header abbreviations is as follows:

- id = atom id
- type = atom type
- nb = number of bonds
- id_1 = atom id of first bond
- id_nb = atom id of Nth bond
- mol = molecule id
- bo_1 = bond order of first bond
- bo_nb = bond order of Nth bond
- abo = atom bond order (sum of all bonds)
- nlp = number of lone pairs
- q = atomic charge

If the filename ends with ".gz", the output file is written in gzipped format. A gzipped dump file will be about 3x smaller than the text version, but will also take longer to write.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in *Speed* of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See *Speed* of the manual for more instructions on how to use the accelerated styles effectively.

16.187.4 Restrictions

The fix reax/c/bonds command requires that the *pair_style reax/c* is invoked. This fix is part of the USER-REAXC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

To write gzipped bond files, you must compile LAMMPS with the -DLAMMPS_GZIP option.

16.187.5 Related commands

pair_style reax/c, *fix reax/c/species*

Default: none

16.188 fix reax/c/species command

16.189 fix reax/c/species/kk command

16.189.1 Syntax

```
fix ID group-ID reax/c/species Nevery Nrepeat Nfreq filename keyword value ...
```

- ID, group-ID are documented in *fix* command
- reax/c/species = style name of this command
- Nevery = sample bond-order every this many timesteps
- Nrepeat = # of bond-order samples used for calculating averages
- Nfreq = calculate average bond-order every this many timesteps
- filename = name of output file
- zero or more keyword/value pairs may be appended
- keyword = *cutoff* or *element* or *position*

```
cutoff value = I J Cutoff
  I, J = atom types
  Cutoff = Bond-order cutoff value for this pair of atom types
element value = Element1, Element2, ...
position value = posfreq filepos
  posfreq = write position files every this many timestep
  filepos = name of position output file
```

16.189.2 Examples

```
fix 1 all reax/c/species 10 10 100 species.out
fix 1 all reax/c/species 1 2 20 species.out cutoff 1 1 0.40 cutoff 1 2 0.55
fix 1 all reax/c/species 1 100 100 species.out element Au O H position 1000 AuOH.pos
```

16.189.3 Description

Write out the chemical species information computed by the ReaxFF potential specified by *pair_style reax/c*. Bond-order values (either averaged or instantaneous, depending on value of *Nrepeat*) are used to determine chemical bonds. Every *Nfreq* timesteps, chemical species information is written to *filename* as a two line output. The first line is a header containing labels. The second line consists of the following: timestep, total number of molecules, total number of distinct species, number of molecules of each species. In this context, "species" means a unique molecule. The chemical formula of each species is given in the first line.

If the filename ends with ".gz", the output file is written in gzipped format. A gzipped dump file will be about 3x smaller than the text version, but will also take longer to write.

Optional keyword *cutoff* can be assigned to change the minimum bond-order values used in identifying chemical bonds between pairs of atoms. Bond-order cutoffs should be carefully chosen, as bond-order cutoffs that are too small may include too many bonds (which will result in an error), while cutoffs that are too large will result in fragmented molecules. The default cutoff of 0.3 usually gives good results.

The optional keyword *element* can be used to specify the chemical symbol printed for each LAMMPS atom type. The number of symbols must match the number of LAMMPS atom types and each symbol must consist of 1 or 2 alphanumeric characters. Normally, these symbols should be chosen to match the chemical identity of each LAMMPS atom type, as specified using the *reax/c pair_coeff* command and the ReaxFF force field file.

The optional keyword *position* writes center-of-mass positions of each identified molecules to file *filepos* every *posfreq* timesteps. The first line contains information on timestep, total number of molecules, total number of distinct species, and box dimensions. The second line is a header containing labels. From the third line downward, each molecule writes a line of output containing the following information: molecule ID, number of atoms in this molecule, chemical formula, total charge, and center-of-mass xyz positions of this molecule. The xyz positions are in fractional coordinates relative to the box dimensions.

For the keyword *position*, the *filepos* is the name of the output file. It can contain the wildcard character "*". If the "*" character appears in *filepos*, then one file per snapshot is written at *posfreq* and the "*" character is replaced with the timestep value. For example, AuO.pos.* becomes AuO.pos.0, AuO.pos.1000, etc.

The *Nevery*, *Nrepeat*, and *Nfreq* arguments specify on what timesteps the bond-order values are sampled to get the average bond order. The species analysis is performed using the average bond-order on timesteps that are a multiple of *Nfreq*. The average is over *Nrepeat* bond-order samples, computed in the preceding portion of the simulation every *Nevery* timesteps. *Nfreq* must be a multiple of *Nevery* and *Nevery* must be non-zero even if *Nrepeat* is 1. Also, the timesteps contributing to the average bond-order cannot overlap, i.e. Nrepeat*Nevery can not exceed Nfreq.

For example, if Nevery=2, Nrepeat=6, and Nfreq=100, then bond-order values on timesteps 90,92,94,96,98,100 will be used to compute the average bond-order for the species analysis output on timestep 100.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix computes both a global vector of length 2 and a per-atom vector, either of which can be accessed by various *output commands*. The values in the global vector are "intensive".

The 2 values in the global vector are as follows:

- 1 = total number of molecules
- 2 = total number of distinct species

The per-atom vector stores the molecule ID for each atom as identified by the fix. If an atom is not in a molecule, its ID will be 0. For atoms in the same molecule, the molecule ID for all of them will be the same and will be equal to the smallest atom ID of any atom in the molecule.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in *Speed* of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See *Speed* of the manual for more instructions on how to use the accelerated styles effectively.

16.189.4 Restrictions

The "fix reax/c/species" currently only works with *pair_style reax/c* and it requires that the *pair_style reax/c* be invoked. This fix is part of the USER-REAXC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

To write gzipped species files, you must compile LAMMPS with the -DLAMMPS_GZIP option.

It should be possible to extend it to other reactive pair_styles (such as *rebo*, *airebo*, *comb*, and *bop*), but this has not yet been done.

16.189.5 Related commands

pair_style reax/c, *fix reax/c/bonds*

16.189.6 Default

The default values for bond-order cutoffs are 0.3 for all I-J pairs. The default element symbols are C, H, O, N. Position files are not written by default.

16.190 fix recenter command

16.190.1 Syntax

```
fix ID group-ID recenter x y z keyword value ...
```

- ID, group-ID are documented in *fix* command
- recenter = style name of this fix command
- x,y,z = constrain center-of-mass to these coords (distance units), any coord can also be NULL or INIT (see below)
- zero or more keyword/value pairs may be appended
- keyword = *shift* or *units*

```
shift value = group-ID
  group-ID = group of atoms whose coords are shifted
units value = box or lattice or fraction
```

16.190.2 Examples

```
fix 1 all recenter 0.0 0.5 0.0
fix 1 all recenter INIT INIT NULL
fix 1 all recenter INIT 0.0 0.0 units box
```

16.190.3 Description

Constrain the center-of-mass position of a group of atoms by adjusting the coordinates of the atoms every timestep. This is simply a small shift that does not alter the dynamics of the system or change the relative coordinates of any pair of atoms in the group. This can be used to insure the entire collection of atoms (or a portion of them) do not drift during the simulation due to random perturbations (e.g. *fix langevin* thermostatting).

Distance units for the x,y,z values are determined by the setting of the *units* keyword, as discussed below. One or more x,y,z values can also be specified as NULL, which means exclude that dimension from this operation. Or it can be specified as INIT which means to constrain the center-of-mass to its initial value at the beginning of the run.

The center-of-mass (COM) is computed for the group specified by the fix. If the current COM is different than the specified x,y,z, then a group of atoms has their coordinates shifted by the difference. By default the shifted group is also the group specified by the fix. A different group can be shifted by using the *shift* keyword. For example, the COM could be computed on a protein to keep it in the center of the simulation box. But the entire system (protein + water) could be shifted.

If the *units* keyword is set to *box*, then the distance units of x,y,z are defined by the *units* command - e.g. Angstroms for *real* units. A *lattice* value means the distance units are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacing. A *fraction* value means a fractional distance between the lo/hi box boundaries, e.g. 0.5 = middle of the box. The default is to use lattice units.

Note that the *velocity* command can be used to create velocities with zero aggregate linear and/or angular momentum.

Note: This fix performs its operations at the same point in the timestep as other time integration fixes, such as *fix nve*, *fix nvt*, or *fix npt*. Thus fix recenter should normally be the last such fix specified in the input script, since the

adjustments it makes to atom coordinates should come after the changes made by time integration. LAMMPS will warn you if your fixes are not ordered this way.

Note: If you use this fix on a small group of atoms (e.g. a molecule in solvent) without using the *shift* keyword to adjust the positions of all atoms in the system, then the results can be unpredictable. For example, if the molecule is pushed consistently in one direction by a flowing solvent, its velocity will increase. But its coordinates will be re-centered, meaning it is moved back towards the force. Thus over time, the velocity and effective temperature of the molecule could become very large, though it won't actually be moving due to the re-centering. If you are thermostatting the entire system, then the solvent would be cooled to compensate. A better solution for this simulation scenario is to use the *fix spring* command to tether the molecule in place.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the distance the group is moved by fix recenter.

This fix also computes global 3-vector which can be accessed by various *output commands*. The 3 quantities in the vector are xyz components of displacement applied to the group of atoms by the fix.

The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.190.4 Restrictions

This fix should not be used with an x,y,z setting that causes a large shift in the system on the 1st timestep, due to the requested COM being very different from the initial COM. This could cause atoms to be lost, especially in parallel. Instead, use the *displace_atoms* command, which can be used to move atoms a large distance.

16.190.5 Related commands

fix momentum, *velocity*

16.190.6 Default

The option defaults are shift = fix group-ID, and units = lattice.

16.191 fix restrain command

16.191.1 Syntax

```
fix ID group-ID restrain keyword args ...
```

- ID, group-ID are documented in *fix* command
- restrain = style name of this fix command
- one or more keyword/arg pairs may be appended

- keyword = *bond* or *angle* or *dihedral*

```
bond args = atom1 atom2 Kstart Kstop r0
  atom1,atom2 = IDs of 2 atoms in bond
  Kstart,Kstop = restraint coefficients at start/end of run (energy units)
  r0 = equilibrium bond distance (distance units)
angle args = atom1 atom2 atom3 Kstart Kstop theta0
  atom1,atom2,atom3 = IDs of 3 atoms in angle, atom2 = middle atom
  Kstart,Kstop = restraint coefficients at start/end of run (energy units)
  theta0 = equilibrium angle theta (degrees)
dihedral args = atom1 atom2 atom3 atom4 Kstart Kstop phi0 keyword/value
  atom1,atom2,atom3,atom4 = IDs of 4 atoms in dihedral in linear order
  Kstart,Kstop = restraint coefficients at start/end of run (energy units)
  phi0 = equilibrium dihedral angle phi (degrees)
  keyword/value = optional keyword value pairs. supported keyword/value␣
↪pairs:
    mult n = dihedral multiplicity n (integer >= 0, default = 1)
```

16.191.2 Examples

```
fix holdem all restrain bond 45 48 2000.0 2000.0 2.75
fix holdem all restrain dihedral 1 2 3 4 2000.0 2000.0 120.0
fix holdem all restrain bond 45 48 2000.0 2000.0 2.75 dihedral 1 2 3 4 2000.0 2000.0␣
↪120.0
fix texas_holdem all restrain dihedral 1 2 3 4 0.0 2000.0 120.0 dihedral 1 2 3 5 0.0␣
↪2000.0 -120.0 dihedral 1 2 3 6 0.0 2000.0 0.0
```

16.191.3 Description

Restrain the motion of the specified sets of atoms by making them part of a bond or angle or dihedral interaction whose strength can vary over time during a simulation. This is functionally similar to creating a bond or angle or dihedral for the same atoms in a data file, as specified by the *read_data* command, albeit with a time-varying pre-factor coefficient, and except for exclusion rules, as explained below.

For the purpose of force field parameter-fitting or mapping a molecular potential energy surface, this fix reduces the hassle and risk associated with modifying data files. In other words, use this fix to temporarily force a molecule to adopt a particular conformation. To create a permanent bond or angle or dihedral, you should modify the data file.

Note: Adding a bond/angle/dihedral with this command does not apply the exclusion rules and weighting factors specified by the *special_bonds* command to atoms in the restraint that are now bonded (1-2,1-3,1-4 neighbors) as a result. If they are close enough to interact in a *pair_style* sense (non-bonded interaction), then the bond/angle/dihedral restraint interaction will simply be superposed on top of that interaction.

The group-ID specified by this fix is ignored.

The second example above applies a restraint to hold the dihedral angle formed by atoms 1, 2, 3, and 4 near 120 degrees using a constant restraint coefficient. The fourth example applies similar restraints to multiple dihedral angles using a restraint coefficient that increases from 0.0 to 2000.0 over the course of the run.

Note: Adding a force to atoms implies a change in their potential energy as they move due to the applied force field. For dynamics via the *run* command, this energy can be added to the system's potential energy for thermodynamic

output (see below). For energy minimization via the *minimize* command, this energy must be added to the system's potential energy to formulate a self-consistent minimization problem (see below).

In order for a restraint to be effective, the restraint force must typically be significantly larger than the forces associated with conventional force field terms. If the restraint is applied during a dynamics run (as opposed to during an energy minimization), a large restraint coefficient can significantly reduce the stable timestep size, especially if the atoms are initially far from the preferred conformation. You may need to experiment to determine what value of K works best for a given application.

For the case of finding a minimum energy structure for a single molecule with particular restraints (e.g. for fitting force field parameters or constructing a potential energy surface), commands such as the following may be useful:

```
# minimize molecule energy with restraints
velocity all create 600.0 8675309 mom yes rot yes dist gaussian
fix NVE all nve
fix TFIX all langevin 600.0 0.0 100 24601
fix REST all restrain dihedral 2 1 3 8 0.0 5000.0 ${angle1} dihedral 3 1 2 9 0.0 5000.
↪0 ${angle2}
fix_modify REST energy yes
run 10000
fix TFIX all langevin 0.0 0.0 100 24601
fix REST all restrain dihedral 2 1 3 8 5000.0 5000.0 ${angle1} dihedral 3 1 2 9 5000.
↪0 5000.0 ${angle2}
fix_modify REST energy yes
run 10000
# sanity check for convergence
minimize 1e-6 1e-9 1000 100000
# report unrestrained energies
unfix REST
run 0
```

The *bond* keyword applies a bond restraint to the specified atoms using the same functional form used by the *bond_style harmonic* command. The potential associated with the restraint is

$$E = K(r - r_0)^2$$

with the following coefficients:

- K (energy/distance^2)
- r_0 (distance)

K and r_0 are specified with the fix. Note that the usual 1/2 factor is included in K.

The *angle* keyword applies an angle restraint to the specified atoms using the same functional form used by the *angle_style harmonic* command. The potential associated with the restraint is

$$E = K(\theta - \theta_0)^2$$

with the following coefficients:

- K (energy/radian^2)
- θ_0 (degrees)

K and θ_0 are specified with the fix. Note that the usual 1/2 factor is included in K.

The *dihedral* keyword applies a dihedral restraint to the specified atoms using a simplified form of the function used by the *dihedral_style charmm* command. The potential associated with the restraint is

$$E = K[1 + \cos(n\phi - d)]$$

with the following coefficients:

- K (energy)
- n (multiplicity, >= 0)
- d (degrees) = $\phi_0 + 180$

K and ϕ_0 are specified with the fix. Note that the value of the dihedral multiplicity n is set by default to 1. You can use the optional *mult* keyword to set it to a different positive integer. Also note that the energy will be a minimum when the current dihedral angle ϕ is equal to ϕ_0.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify* *energy* option is supported by this fix to add the potential energy associated with this fix to the system's potential energy as part of *thermodynamic output*.

The *fix_modify* *respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix is adding its forces. Default is the outermost level.

Note: If you want the fictitious potential energy associated with the added forces to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the *fix_modify* *energy* option for this fix.

This fix computes a global scalar and a global vector of length 3, which can be accessed by various *output commands*. The scalar is the total potential energy for *all* the restraints as discussed above. The vector values are the sum of contributions to the following individual categories:

- 1 = bond energy
- 2 = angle energy
- 3 = dihedral energy

The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

16.191.4 Restrictions

none

Related commands: none

Default: none

16.192 fix rhok command

```
fix ID group-ID rhok nx ny nz K a
```

- ID, group-ID are documented in *fix* command
- nx, ny, nz = k-vector of collective density field
- K = spring constant of bias potential
- a = anchor point of bias potential

16.192.1 Examples

```
fix bias all rhok 16 0 0 4.0 16.0
fix 1 all npt temp 0.8 0.8 4.0 z 2.2 2.2 8.0
# output of 4 values from fix rhok: U_bias rho_k_RE  rho_k_IM  |rho_k|
thermo_style custom step temp pzz lz f_bias f_bias[1] f_bias[2] f_bias[3]
```

16.192.2 Description

The fix applies a force to atoms given by the potential

$$
\begin{aligned}
U =& \frac{1}{2} K (|\rho_{\vec{k}}| - a)^2 \\
\rho_{\vec{k}} =& \sum_j^N \exp(-i\vec{k} \cdot \vec{r}_j)/\sqrt{N} \\
\vec{k} =& (2\pi n_x/L_x, 2\pi n_y/L_y, 2\pi n_z/L_z)
\end{aligned}
$$

as described in *(Pedersen)*.

This field, which biases configurations with long-range order, can be used to study crystal-liquid interfaces and determine melting temperatures *(Pedersen)*.

An example of using the interface pinning method is located in the *examples/USER/misc/rhok* directory.

16.192.3 Restrictions

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.192.4 Related commands

thermo_style

Default: none

(Pedersen) Pedersen, J. Chem. Phys., 139, 104102 (2013).

16.193 fix rigid command

16.194 fix rigid/omp command

16.195 fix rigid/nve command

16.196 fix rigid/nve/omp command

16.197 fix rigid/nvt command

16.198 fix rigid/nvt/omp command

16.199 fix rigid/npt command

16.200 fix rigid/npt/omp command

16.201 fix rigid/nph command

16.202 fix rigid/nph/omp command

16.203 fix rigid/small command

16.204 fix rigid/small/omp command

16.205 fix rigid/nve/small command

16.206 fix rigid/nvt/small command

16.207 fix rigid/npt/small command

16.208 fix rigid/nph/small command

16.208.1 Syntax

```
fix ID group-ID style bodystyle args keyword values ...
```

- ID, group-ID are documented in *fix* command
- style = *rigid* or *rigid/nve* or *rigid/nvt* or *rigid/npt* or *rigid/nph* or *rigid/small* or *rigid/nve/small* or *rigid/nvt/small* or *rigid/npt/small* or *rigid/nph/small*

- bodystyle = *single* or *molecule* or *group*

```
single args = none
molecule args = none
custom args = i_propname or v_varname
  i_propname = an integer property defined via fix property/atom
  v_varname  = an atom-style or atomfile-style variable
group args = N groupID1 groupID2 ...
  N = # of groups
  groupID1, groupID2, ... = list of N group IDs
```

- zero or more keyword/value pairs may be appended
- keyword = *langevin* or *reinit* or *temp* or *iso* or *aniso* or *x* or *y* or *z* or *couple* or *tparam* or *pchain* or *dilate* or *force* or *torque* or *infile*

```
langevin values = Tstart Tstop Tperiod seed
  Tstart,Tstop = desired temperature at start/stop of run (temperature␣
↪units)
  Tdamp = temperature damping parameter (time units)
  seed = random number seed to use for white noise (positive integer)
reinit = yes or no
temp values = Tstart Tstop Tdamp
  Tstart,Tstop = desired temperature at start/stop of run (temperature␣
↪units)
  Tdamp = temperature damping parameter (time units)
iso or aniso values = Pstart Pstop Pdamp
  Pstart,Pstop = scalar external pressure at start/end of run (pressure␣
↪units)
  Pdamp = pressure damping parameter (time units)
x or y or z values = Pstart Pstop Pdamp
  Pstart,Pstop = external stress tensor component at start/end of run␣
↪(pressure units)
  Pdamp = stress damping parameter (time units)
couple = none or xyz or xy or yz or xz
tparam values = Tchain Titer Torder
  Tchain = length of Nose/Hoover thermostat chain
  Titer = number of thermostat iterations performed
  Torder = 3 or 5 = Yoshida-Suzuki integration parameters
pchain values = Pchain
  Pchain = length of the Nose/Hoover thermostat chain coupled with the␣
↪barostat
dilate value = dilate-group-ID
  dilate-group-ID = only dilate atoms in this group due to barostat␣
↪volume changes
force values = M xflag yflag zflag
  M = which rigid body from 1-Nbody (see asterisk form below)
  xflag,yflag,zflag = off/on if component of center-of-mass force is␣
↪active
torque values = M xflag yflag zflag
  M = which rigid body from 1-Nbody (see asterisk form below)
  xflag,yflag,zflag = off/on if component of center-of-mass torque is␣
↪active
infile filename
  filename = file with per-body values of mass, center-of-mass, moments␣
↪of inertia
```

```
mol value = template-ID
  template-ID = ID of molecule template specified in a separate molecule␣
↪command
```

16.208.2 Examples

```
fix 1 clump rigid single reinit yes
fix 1 clump rigid/small molecule
fix 1 clump rigid single force 1 off off on langevin 1.0 1.0 1.0 428984
fix 1 polychains rigid/nvt molecule temp 1.0 1.0 5.0 reinit no
fix 1 polychains rigid molecule force 1*5 off off off force 6*10 off off on
fix 1 polychains rigid/small molecule langevin 1.0 1.0 1.0 428984
fix 2 fluid rigid group 3 clump1 clump2 clump3 torque * off off off
fix 1 rods rigid/npt molecule temp 300.0 300.0 100.0 iso 0.5 0.5 10.0
fix 1 particles rigid/npt molecule temp 1.0 1.0 5.0 x 0.5 0.5 1.0 z 0.5 0.5 1.
↪0 couple xz
fix 1 water rigid/nph molecule iso 0.5 0.5 1.0
fix 1 particles rigid/npt/small molecule temp 1.0 1.0 1.0 iso 0.5 0.5 1.0

variable bodyid atom 1.0*gmask(clump1)+2.0*gmask(clump2)+3.0*gmask(clump3)
fix 1 clump rigid custom v_bodyid

variable bodyid atomfile bodies.txt
fix 1 clump rigid custom v_bodyid

fix 0 all property/atom i_bodyid
read_restart data.rigid fix 0 NULL Bodies
fix 1 clump rigid/small custom i_bodyid
```

16.208.3 Description

Treat one or more sets of atoms as independent rigid bodies. This means that each timestep the total force and torque on each rigid body is computed as the sum of the forces and torques on its constituent particles. The coordinates, velocities, and orientations of the atoms in each body are then updated so that the body moves and rotates as a single entity. This is implemented by creating internal data structures for each rigid body and performing time integration on these data structures. Positions, velocities, and orientations of the constituent particles are regenerated from the rigid body data structures in every time step. This restricts which operations and fixes can be applied to rigid bodies. See below for a detailed discussion.

Examples of large rigid bodies are a colloidal particle, or portions of a biomolecule such as a protein.

Example of small rigid bodies are patchy nanoparticles, such as those modeled in *this paper* by Sharon Glotzer's group, clumps of granular particles, lipid molecules consisting of one or more point dipoles connected to other spheroids or ellipsoids, irregular particles built from line segments (2d) or triangles (3d), and coarse-grain models of nano or colloidal particles consisting of a small number of constituent particles. Note that the *fix shake* command can also be used to rigidify small molecules of 2, 3, or 4 atoms, e.g. water molecules. That fix treats the constituent atoms as point masses.

These fixes also update the positions and velocities of the atoms in each rigid body via time integration, in the NVE, NVT, NPT, or NPH ensemble, as described below.

There are two main variants of this fix, fix rigid and fix rigid/small. The NVE/NVT/NPT/NHT versions belong to one of the two variants, as their style names indicate.

Note: Not all of the *bodystyle* options and keyword/value options are available for both the *rigid* and *rigid/small* variants. See details below.

The *rigid* styles are typically the best choice for a system with a small number of large rigid bodies, each of which can extend across the domain of many processors. It operates by creating a single global list of rigid bodies, which all processors contribute to. MPI_Allreduce operations are performed each timestep to sum the contributions from each processor to the force and torque on all the bodies. This operation will not scale well in parallel if large numbers of rigid bodies are simulated.

The *rigid/small* styles are typically best for a system with a large number of small rigid bodies. Each body is assigned to the atom closest to the geometrical center of the body. The fix operates using local lists of rigid bodies owned by each processor and information is exchanged and summed via local communication between neighboring processors when ghost atom info is accumulated.

Note: To use the *rigid/small* styles the ghost atom cutoff must be large enough to span the distance between the atom that owns the body and every other atom in the body. This distance value is printed out when the rigid bodies are defined. If the *pair_style* cutoff plus neighbor skin does not span this distance, then you should use the *comm_modify cutoff* command with a setting epsilon larger than the distance.

Which of the two variants is faster for a particular problem is hard to predict. The best way to decide is to perform a short test run. Both variants should give identical numerical answers for short runs. Long runs should give statistically similar results, but round-off differences may accumulate to produce divergent trajectories.

Note: You should not update the atoms in rigid bodies via other time-integration fixes (e.g. *fix nve*, *fix nvt*, *fix npt*, *fix move*), or you will have conflicting updates to positions and velocities resulting in unphysical behavior in most cases. When performing a hybrid simulation with some atoms in rigid bodies, and some not, a separate time integration fix like *fix nve* or *fix nvt* should be used for the non-rigid particles.

Note: These fixes are overkill if you simply want to hold a collection of atoms stationary or have them move with a constant velocity. A simpler way to hold atoms stationary is to not include those atoms in your time integration fix. E.g. use "fix 1 mobile nve" instead of "fix 1 all nve", where "mobile" is the group of atoms that you want to move. You can move atoms with a constant velocity by assigning them an initial velocity (via the *velocity* command), setting the force on them to 0.0 (via the *fix setforce* command), and integrating them as usual (e.g. via the *fix nve* command).

Warning: The aggregate properties of each rigid body are calculated at the start of a simulation run and are maintained in internal data structures. The properties include the position and velocity of the center-of-mass of the body, its moments of inertia, and its angular momentum. This is done using the properties of the constituent atoms of the body at that point in time (or see the *infile* keyword option). Thereafter, changing these properties of individual atoms in the body will have no effect on a rigid body's dynamics, unless they effect any computation of per-atom forces or torques. If the keyword *reinit* is set to *yes* (the default), the rigid body data structures will be recreated at the beginning of each *run* command; if the keyword *reinit* is set to *no*, the rigid body data structures will be built only at the very first *run* command and maintained for as long as the rigid fix is defined. For example, you might think you could displace the atoms in a body or add a large velocity to each atom in a body to make it move in a desired direction before a 2nd run is performed, using the *set* or *displace_atoms* or *velocity* commands. But these commands will not affect the internal attributes of the body unless *reinit* is set to *yes*. With *reinit* set to *no* (or using the *infile* option, which implies *reinit no*) the position and velocity of individual atoms in the body will be reset when time integration starts again.

Each rigid body must have two or more atoms. An atom can belong to at most one rigid body. Which atoms are in which bodies can be defined via several options.

Note: With the *rigid/small* styles, which require that *bodystyle* be specified as *molecule* or *custom*, you can define a system that has no rigid bodies initially. This is useful when you are using the *mol* keyword in conjunction with another fix that is adding rigid bodies on-the-fly as molecules, such as *fix deposit* or *fix pour*.

For bodystyle *single* the entire fix group of atoms is treated as one rigid body. This option is only allowed for the *rigid* styles.

For bodystyle *molecule*, atoms are grouped into rigid bodies by their respective molecule IDs: each set of atoms in the fix group with the same molecule ID is treated as a different rigid body. This option is allowed for both the *rigid* and *rigid/small* styles. Note that atoms with a molecule ID = 0 will be treated as a single rigid body. For a system with atomic solvent (typically this is atoms with molecule ID = 0) surrounding rigid bodies, this may not be what you want. Thus you should be careful to use a fix group that only includes atoms you want to be part of rigid bodies.

Bodystyle *custom* is similar to bodystyle *molecule* except that it is more flexible in using other per-atom properties to define the sets of atoms that form rigid bodies. An integer vector defined by the *fix property/atom* command can be used. Or an *atom-style or atomfile-style variable* can be used; the floating-point value produced by the variable is rounded to an integer. As with bodystyle *molecule*, each set of atoms in the fix groups with the same integer value is treated as a different rigid body. Since fix property/atom vectors and atom-style variables produce values for all atoms, you should be careful to use a fix group that only includes atoms you want to be part of rigid bodies.

Note: To compute the initial center-of-mass position and other properties of each rigid body, the image flags for each atom in the body are used to "unwrap" the atom coordinates. Thus you must insure that these image flags are consistent so that the unwrapping creates a valid rigid body (one where the atoms are close together), particularly if the atoms in a single rigid body straddle a periodic boundary. This means the input data file or restart file must define the image flags for each atom consistently or that you have used the *set* command to specify them correctly. If a dimension is non-periodic then the image flag of each atom must be 0 in that dimension, else an error is generated.

The *force* and *torque* keywords discussed next are only allowed for the *rigid* styles.

By default, each rigid body is acted on by other atoms which induce an external force and torque on its center of mass, causing it to translate and rotate. Components of the external center-of-mass force and torque can be turned off by the *force* and *torque* keywords. This may be useful if you wish a body to rotate but not translate, or vice versa, or if you wish it to rotate or translate continuously unaffected by interactions with other particles. Note that if you expect a rigid body not to move or rotate by using these keywords, you must insure its initial center-of-mass translational or angular velocity is 0.0. Otherwise the initial translational or angular momentum the body has will persist.

An xflag, yflag, or zflag set to *off* means turn off the component of force of torque in that dimension. A setting of *on* means turn on the component, which is the default. Which rigid body(s) the settings apply to is determined by the first argument of the *force* and *torque* keywords. It can be an integer M from 1 to Nbody, where Nbody is the number of rigid bodies defined. A wild-card asterisk can be used in place of, or in conjunction with, the M argument to set the flags for multiple rigid bodies. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of rigid bodies, then an asterisk with no numeric values means all bodies from 1 to N. A leading asterisk means all bodies from 1 to n (inclusive). A trailing asterisk means all bodies from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). Note that you can use the *force* or *torque* keywords as many times as you like. If a particular rigid body has its component flags set multiple times, the settings from the final keyword are used.

Note: For computational efficiency, you may wish to turn off pairwise and bond interactions within each rigid body, as they no longer contribute to the motion. The *neigh_modify exclude* and *delete_bonds* commands are used to do this.

If the rigid bodies have strongly overlapping atoms, you may need to turn off these interactions to avoid numerical problems due to large equal/opposite intra-body forces swamping the contribution of small inter-body forces.

For computational efficiency, you should typically define one fix rigid or fix rigid/small command which includes all the desired rigid bodies. LAMMPS will allow multiple rigid fixes to be defined, but it is more expensive.

The constituent particles within a rigid body can be point particles (the default in LAMMPS) or finite-size particles, such as spheres or ellipsoids or line segments or triangles. See the *atom_style sphere and ellipsoid and line and tri* commands for more details on these kinds of particles. Finite-size particles contribute differently to the moment of inertia of a rigid body than do point particles. Finite-size particles can also experience torque (e.g. due to *frictional granular interactions*) and have an orientation. These contributions are accounted for by these fixes.

Forces between particles within a body do not contribute to the external force or torque on the body. Thus for computational efficiency, you may wish to turn off pairwise and bond interactions between particles within each rigid body. The *neigh_modify exclude* and *delete_bonds* commands are used to do this. For finite-size particles this also means the particles can be highly overlapped when creating the rigid body.

The *rigid*, *rigid/nve*, *rigid/small*, and *rigid/small/nve* styles perform constant NVE time integration. They are referred to below as the 4 NVE rigid styles. The only difference is that the *rigid* and *rigid/small* styles use an integration technique based on Richardson iterations. The *rigid/nve* and *rigid/small/nve* styles uses the methods described in the paper by *Miller*, which are thought to provide better energy conservation than an iterative approach.

The *rigid/nvt* and *rigid/nvt/small* styles performs constant NVT integration using a Nose/Hoover thermostat with chains as described originally in *(Hoover)* and *(Martyna)*, which thermostats both the translational and rotational degrees of freedom of the rigid bodies. They are referred to below as the 2 NVT rigid styles. The rigid-body algorithm used by *rigid/nvt* is described in the paper by *Kamberaj*.

The *rigid/npt*, *rigid/nph*, *rigid/npt/small*, and *rigid/nph/small* styles perform constant NPT or NPH integration using a Nose/Hoover barostat with chains. They are referred to below as the 4 NPT and NPH rigid styles. For the NPT case, the same Nose/Hoover thermostat is also used as with *rigid/nvt* and *rigid/nvt/small*.

The barostat parameters are specified using one or more of the *iso*, *aniso*, *x*, *y*, *z* and *couple* keywords. These keywords give you the ability to specify 3 diagonal components of the external stress tensor, and to couple these components together so that the dimensions they represent are varied together during a constant-pressure simulation. The effects of these keywords are similar to those defined in *fix npt/nph*

Note: Currently the *rigid/npt*, *rigid/nph*, *rigid/npt/small*, and *rigid/nph/small* styles do not support triclinic (non-orthogonal) boxes.

The target pressures for each of the 6 components of the stress tensor can be specified independently via the *x*, *y*, *z* keywords, which correspond to the 3 simulation box dimensions. For each component, the external pressure or tensor component at each timestep is a ramped value during the run from *Pstart* to *Pstop*. If a target pressure is specified for a component, then the corresponding box dimension will change during a simulation. For example, if the *y* keyword is used, the y-box length will change. A box dimension will not change if that component is not specified, although you have the option to change that dimension via the *fix deform* command.

For all barostat keywords, the *Pdamp* parameter operates like the *Tdamp* parameter, determining the time scale on which pressure is relaxed. For example, a value of 10.0 means to relax the pressure in a timespan of (roughly) 10 time units (e.g. tau or fmsec or psec - see the *units* command).

Regardless of what atoms are in the fix group (the only atoms which are time integrated), a global pressure or stress tensor is computed for all atoms. Similarly, when the size of the simulation box is changed, all atoms are re-scaled to new positions, unless the keyword *dilate* is specified with a *dilate-group-ID* for a group that represents a subset

of the atoms. This can be useful, for example, to leave the coordinates of atoms in a solid substrate unchanged and controlling the pressure of a surrounding fluid. Another example is a system consisting of rigid bodies and point particles where the barostat is only coupled with the rigid bodies. This option should be used with care, since it can be unphysical to dilate some atoms and not others, because it can introduce large, instantaneous displacements between a pair of atoms (one dilated, one not) that are far from the dilation origin.

The *couple* keyword allows two or three of the diagonal components of the pressure tensor to be "coupled" together. The value specified with the keyword determines which are coupled. For example, *xz* means the *Pxx* and *Pzz* components of the stress tensor are coupled. *Xyz* means all 3 diagonal components are coupled. Coupling means two things: the instantaneous stress will be computed as an average of the corresponding diagonal components, and the coupled box dimensions will be changed together in lockstep, meaning coupled dimensions will be dilated or contracted by the same percentage every timestep. The *Pstart*, *Pstop*, *Pdamp* parameters for any coupled dimensions must be identical. *Couple xyz* can be used for a 2d simulation; the *z* dimension is simply ignored.

The *iso* and *aniso* keywords are simply shortcuts that are equivalent to specifying several other keywords together.

The keyword *iso* means couple all 3 diagonal components together when pressure is computed (hydrostatic pressure), and dilate/contract the dimensions together. Using "iso Pstart Pstop Pdamp" is the same as specifying these 4 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
couple xyz
```

The keyword *aniso* means *x*, *y*, and *z* dimensions are controlled independently using the *Pxx*, *Pyy*, and *Pzz* components of the stress tensor as the driving forces, and the specified scalar external pressure. Using "aniso Pstart Pstop Pdamp" is the same as specifying these 4 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
couple none
```

The keyword/value option pairs are used in the following ways.

The *reinit* keyword determines, whether the rigid body properties are re-initialized between run commands. With the option *yes* (the default) this is done, with the option *no* this is not done. Turning off the re-initialization can be helpful to protect rigid bodies against unphysical manipulations between runs or when properties cannot be easily re-computed (e.g. when read from a file). When using the *infile* keyword, the *reinit* option is automatically set to *no*.

The *langevin* and *temp* and *tparam* keywords perform thermostatting of the rigid bodies, altering both their translational and rotational degrees of freedom. What is meant by "temperature" of a collection of rigid bodies and how it can be monitored via the fix output is discussed below.

The *langevin* keyword applies a Langevin thermostat to the constant NVE time integration performed by any of the 4 NVE rigid styles: *rigid*, *rigid/nve*, *rigid/small*, *rigid/small/nve*. It cannot be used with the 2 NVT rigid styles: *rigid/nvt*, *rigid/small/nvt*. The desired temperature at each timestep is a ramped value during the run from *Tstart* to *Tstop*. The *Tdamp* parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 100.0 means to relax the temperature in a timespan of (roughly) 100 time units (tau or fmsec or psec - see the *units* command). The random # *seed* must be a positive integer.

The way that Langevin thermostatting operates is explained on the *fix langevin* doc page. If you wish to simply viscously damp the rotational motion without thermostatting, you can set *Tstart* and *Tstop* to 0.0, which means only the viscous drag term in the Langevin thermostat will be applied. See the discussion on the *fix viscous* doc page for details.

Note: When the *langevin* keyword is used with fix rigid versus fix rigid/small, different dynamics will result for parallel runs. This is because of the way random numbers are used in the two cases. The dynamics for the two cases should be statistically similar, but will not be identical, even for a single timestep.

The *temp* and *tparam* keywords apply a Nose/Hoover thermostat to the NVT time integration performed by the 2 NVT rigid styles. They cannot be used with the 4 NVE rigid styles. The desired temperature at each timestep is a ramped value during the run from *Tstart* to *Tstop*. The *Tdamp* parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 100.0 means to relax the temperature in a timespan of (roughly) 100 time units (tau or fmsec or psec - see the *units* command).

Nose/Hoover chains are used in conjunction with this thermostat. The *tparam* keyword can optionally be used to change the chain settings used. *Tchain* is the number of thermostats in the Nose Hoover chain. This value, along with *Tdamp* can be varied to dampen undesirable oscillations in temperature that can occur in a simulation. As a rule of thumb, increasing the chain length should lead to smaller oscillations. The keyword *pchain* specifies the number of thermostats in the chain thermostatting the barostat degrees of freedom.

Note: There are alternate ways to thermostat a system of rigid bodies. You can use *fix langevin* to treat the individual particles in the rigid bodies as effectively immersed in an implicit solvent, e.g. a Brownian dynamics model. For hybrid systems with both rigid bodies and solvent particles, you can thermostat only the solvent particles that surround one or more rigid bodies by appropriate choice of groups in the compute and fix commands for temperature and thermostatting. The solvent interactions with the rigid bodies should then effectively thermostat the rigid body temperature as well without use of the Langevin or Nose/Hoover options associated with the fix rigid commands.

The *mol* keyword can only be used with the *rigid/small* styles. It must be used when other commands, such as *fix deposit* or *fix pour*, add rigid bodies on-the-fly during a simulation. You specify a *template-ID* previously defined using the *molecule* command, which reads a file that defines the molecule. You must use the same *template-ID* that the other fix which is adding rigid bodies uses. The coordinates, atom types, atom diameters, center-of-mass, and moments of inertia can be specified in the molecule file. See the *molecule* command for details. The only settings required to be in this file are the coordinates and types of atoms in the molecule, in which case the molecule command calculates the other quantities itself.

Note that these other fixes create new rigid bodies, in addition to those defined initially by this fix via the *bodystyle* setting.

Also note that when using the *mol* keyword, extra restart information about all rigid bodies is written out whenever a restart file is written out. See the NOTE in the next section for details.

The *infile* keyword allows a file of rigid body attributes to be read in from a file, rather then having LAMMPS compute them. There are 5 such attributes: the total mass of the rigid body, its center-of-mass position, its 6 moments of inertia, its center-of-mass velocity, and the 3 image flags of the center-of-mass position. For rigid bodies consisting of point particles or non-overlapping finite-size particles, LAMMPS can compute these values accurately. However, for rigid bodies consisting of finite-size particles which overlap each other, LAMMPS will ignore the overlaps when computing these 4 attributes. The amount of error this induces depends on the amount of overlap. To avoid this issue, the values can be pre-computed (e.g. using Monte Carlo integration).

The format of the file is as follows. Note that the file does not have to list attributes for every rigid body integrated by fix rigid. Only bodies which the file specifies will have their computed attributes overridden. The file can contain initial blank lines or comment lines starting with "#" which are ignored. The first non-blank, non-comment line should list N = the number of lines to follow. The N successive lines contain the following information:

```
ID1 masstotal xcm ycm zcm ixx iyy izz ixy ixz iyz vxcm vycm vzcm lx ly lz ixcm iycm␣
↪izcm
ID2 masstotal xcm ycm zcm ixx iyy izz ixy ixz iyz vxcm vycm vzcm lx ly lz ixcm iycm␣
↪izcm
...
IDN masstotal xcm ycm zcm ixx iyy izz ixy ixz iyz vxcm vycm vzcm lx ly lz ixcm iycm␣
↪izcm
```

The rigid body IDs are all positive integers. For the *single* bodystyle, only an ID of 1 can be used. For the *group* bodystyle, IDs from 1 to Ng can be used where Ng is the number of specified groups. For the *molecule* bodystyle, use the molecule ID for the atoms in a specific rigid body as the rigid body ID.

The masstotal and center-of-mass coordinates (xcm,ycm,zcm) are self-explanatory. The center-of-mass should be consistent with what is calculated for the position of the rigid body with all its atoms unwrapped by their respective image flags. If this produces a center-of-mass that is outside the simulation box, LAMMPS wraps it back into the box.

The 6 moments of inertia (ixx,iyy,izz,ixy,ixz,iyz) should be the values consistent with the current orientation of the rigid body around its center of mass. The values are with respect to the simulation box XYZ axes, not with respect to the principal axes of the rigid body itself. LAMMPS performs the latter calculation internally.

The (vxcm,vycm,vzcm) values are the velocity of the center of mass. The (lx,ly,lz) values are the angular momentum of the body. The (vxcm,vycm,vzcm) and (lx,ly,lz) values can simply be set to 0 if you wish the body to have no initial motion.

The (ixcm,iycm,izcm) values are the image flags of the center of mass of the body. For periodic dimensions, they specify which image of the simulation box the body is considered to be in. An image of 0 means it is inside the box as defined. A value of 2 means add 2 box lengths to get the true value. A value of -1 means subtract 1 box length to get the true value. LAMMPS updates these flags as the rigid bodies cross periodic boundaries during the simulation.

Note: If you use the *infile* or *mol* keywords and write restart files during a simulation, then each time a restart file is written, the fix also write an auxiliary restart file with the name rfile.rigid, where "rfile" is the name of the restart file, e.g. tmp.restart.10000 and tmp.restart.10000.rigid. This auxiliary file is in the same format described above. Thus it can be used in a new input script that restarts the run and re-specifies a rigid fix using an *infile* keyword and the appropriate filename. Note that the auxiliary file will contain one line for every rigid body, even if the original file only listed a subset of the rigid bodies.

If you use a *temperature compute* with a group that includes particles in rigid bodies, the degrees-of-freedom removed by each rigid body are accounted for in the temperature (and pressure) computation, but only if the temperature group includes all the particles in a particular rigid body.

A 3d rigid body has 6 degrees of freedom (3 translational, 3 rotational), except for a collection of point particles lying on a straight line, which has only 5, e.g a dimer. A 2d rigid body has 3 degrees of freedom (2 translational, 1 rotational).

Note: You may wish to explicitly subtract additional degrees-of-freedom if you use the *force* and *torque* keywords to eliminate certain motions of one or more rigid bodies. LAMMPS does not do this automatically.

The rigid body contribution to the pressure of the system (virial) is also accounted for by this fix.

If your simulation is a hybrid model with a mixture of rigid bodies and non-rigid particles (e.g. solvent) there are several ways these rigid fixes can be used in tandem with *fix nve*, *fix nvt*, *fix npt*, and *fix nph*.

If you wish to perform NVE dynamics (no thermostatting or barostatting), use one of 4 NVE rigid styles to integrate the rigid bodies, and *fix nve* to integrate the non-rigid particles.

If you wish to perform NVT dynamics (thermostatting, but no barostatting), you can use one of the 2 NVT rigid styles for the rigid bodies, and any thermostatting fix for the non-rigid particles (*fix nvt*, *fix langevin*, *fix temp/berendsen*). You can also use one of the 4 NVE rigid styles for the rigid bodies and thermostat them using *fix langevin* on the group that contains all the particles in the rigid bodies. The net force added by *fix langevin* to each rigid body effectively thermostats its translational center-of-mass motion. Not sure how well it does at thermostatting its rotational motion.

If you with to perform NPT or NPH dynamics (barostatting), you cannot use both *fix npt* and the NPT or NPH rigid styles. This is because there can only be one fix which monitors the global pressure and changes the simulation box dimensions. So you have 3 choices:

- Use one of the 4 NPT or NPH styles for the rigid bodies. Use the *dilate* all option so that it will dilate the positions of the non-rigid particles as well. Use *fix nvt* (or any other thermostat) for the non-rigid particles.
- Use *fix npt* for the group of non-rigid particles. Use the *dilate* all option so that it will dilate the center-of-mass positions of the rigid bodies as well. Use one of the 4 NVE or 2 NVT rigid styles for the rigid bodies.
- Use *fix press/berendsen* to compute the pressure and change the box dimensions. Use one of the 4 NVE or 2 NVT rigid styles for the rigid bodies. Use *fix nvt* (or any other thermostat) for the non-rigid particles.

In all case, the rigid bodies and non-rigid particles both contribute to the global pressure and the box is scaled the same by any of the barostatting fixes.

You could even use the 2nd and 3rd options for a non-hybrid simulation consisting of only rigid bodies, assuming you give *fix npt* an empty group, though it's an odd thing to do. The barostatting fixes (*fix npt* and *fix press/berensen*) will monitor the pressure and change the box dimensions, but not time integrate any particles. The integration of the rigid bodies will be performed by fix rigid/nvt.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about the 4 NVE rigid styles is written to *binary restart files*. The exception is if the *infile* or *mol* keyword is used, in which case an auxiliary file is written out with rigid body information each time a restart file is written, as explained above for the *infile* keyword. For the 2 NVT rigid styles, the state of the Nose/Hoover thermostat is written to *binary restart files*. Ditto for the 4 NPT and NPH rigid styles, and the state of the Nose/Hoover barostat. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify* *energy* option is supported by the 6 NVT, NPT, NPH rigid styles to add the energy change induced by the thermostatting to the system's potential energy as part of *thermodynamic output*.

The *fix_modify* *virial* option is supported by this fix to add the contribution due to keeping the objects rigid to the system's virial as part of *thermodynamic output*. The default is *virial yes*

The *fix_modify* *temp* and *press* options are supported by the 4 NPT and NPH rigid styles to change the computes used to calculate the instantaneous pressure tensor. Note that the 2 NVT rigid fixes do not use any external compute to compute instantaneous temperature.

The *fix_modify* *bodyforces* option is supported by all rigid styles to set whether per-body forces and torques are computed early or late in a timestep, i.e. at the post-force stage or at the final-integrate stage or the timestep, respectively.

The 2 NVE rigid fixes compute a global scalar which can be accessed by various *output commands*. The scalar value calculated by these fixes is "intensive". The scalar is the current temperature of the collection of rigid bodies. This is averaged over all rigid bodies and their translational and rotational degrees of freedom. The translational energy of a rigid body is 1/2 m v^2, where m = total mass of the body and v = the velocity of its center of mass. The rotational energy of a rigid body is 1/2 I w^2, where I = the moment of inertia tensor of the body and w = its angular velocity. Degrees of freedom constrained by the *force* and *torque* keywords are removed from this calculation, but only for the *rigid* and *rigid/nve* fixes.

The 6 NVT, NPT, NPH rigid fixes compute a global scalar which can be accessed by various *output commands*. The scalar value calculated by these fixes is "extensive". The scalar is the cumulative energy change due to the thermostatting and barostatting the fix performs.

All of the *rigid* styles (not the *rigid/small* styles) compute a global array of values which can be accessed by various *output commands*. Similar information about the bodies defined by the *rigid/small* styles can be accessed via the *compute rigid/local* command.

The number of rows in the array is equal to the number of rigid bodies. The number of columns is 15. Thus for each rigid body, 15 values are stored: the xyz coords of the center of mass (COM), the xyz components of the COM velocity, the xyz components of the force acting on the COM, the xyz components of the torque acting on the COM, and the xyz image flags of the COM.

The center of mass (COM) for each body is similar to unwrapped coordinates written to a dump file. It will always be inside (or slightly outside) the simulation box. The image flags have the same meaning as image flags for atom positions (see the "dump" command). This means you can calculate the unwrapped COM by applying the image flags to the COM, the same as when unwrapped coordinates are written to a dump file.

The force and torque values in the array are not affected by the *force* and *torque* keywords in the fix rigid command; they reflect values before any changes are made by those keywords.

The ordering of the rigid bodies (by row in the array) is as follows. For the *single* keyword there is just one rigid body. For the *molecule* keyword, the bodies are ordered by ascending molecule ID. For the *group* keyword, the list of group IDs determines the ordering of bodies.

The array values calculated by these fixes are "intensive", meaning they are independent of the number of atoms in the simulation.

No parameter of these fixes can be used with the *start/stop* keywords of the *run* command. These fixes are not invoked during *energy minimization*.

16.208.4 Restrictions

These fixes are all part of the RIGID package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Assigning a temperature via the *velocity create* command to a system with *rigid bodies* may not have the desired outcome for two reasons. First, the velocity command can be invoked before the rigid-body fix is invoked or initialized and the number of adjusted degrees of freedom (DOFs) is known. Thus it is not possible to compute the target temperature correctly. Second, the assigned velocities may be partially canceled when constraints are first enforced, leading to a different temperature than desired. A workaround for this is to perform a *run 0* command, which insures all

DOFs are accounted for properly, and then rescale the temperature to the desired value before performing a simulation. For example:

```
velocity all create 300.0 12345
run 0                           # temperature may not be 300K
velocity all scale 300.0        # now it should be
```

16.208.5 Related commands

delete_bonds, *neigh_modify* exclude, *fix shake*

16.208.6 Default

The option defaults are force * on on on and torque * on on on, meaning all rigid bodies are acted on by center-of-mass force and torque. Also Tchain = Pchain = 10, Titer = 1, Torder = 3, reinit = yes.

(Hoover) Hoover, Phys Rev A, 31, 1695 (1985).

(Kamberaj) Kamberaj, Low, Neal, J Chem Phys, 122, 224114 (2005).

(Martyna) Martyna, Klein, Tuckerman, J Chem Phys, 97, 2635 (1992); Martyna, Tuckerman, Tobias, Klein, Mol Phys, 87, 1117.

(Miller) Miller, Eleftheriou, Pattnaik, Ndirango, and Newns, J Chem Phys, 116, 8649 (2002).

(Zhang) Zhang, Glotzer, Nanoletters, 4, 1407-1413 (2004).

16.209 fix rigid/meso command

16.209.1 Syntax

```
fix ID group-ID rigid/meso bodystyle args keyword values ...
```

- ID, group-ID are documented in *fix* command
- rigid/meso = style name of this fix command
- bodystyle = *single* or *molecule* or *group*

```
single args = none
molecule args = none
custom args = i_propname or v_varname
  i_propname = an integer property defined via fix property/atom
  v_varname  = an atom-style or atomfile-style variable
group args = N groupID1 groupID2 ...
  N = # of groups
  groupID1, groupID2, ... = list of N group IDs
```

- zero or more keyword/value pairs may be appended
- keyword = *reinit* or *force* or *torque* or *infile*

```
reinit = yes or no
force values = M xflag yflag zflag
  M = which rigid body from 1-Nbody (see asterisk form below)
  xflag,yflag,zflag = off/on if component of center-of-mass force is␣
↪active
torque values = M xflag yflag zflag
  M = which rigid body from 1-Nbody (see asterisk form below)
  xflag,yflag,zflag = off/on if component of center-of-mass torque is␣
↪active
infile filename
  filename = file with per-body values of mass, center-of-mass, moments␣
↪of inertia
```

16.209.2 Examples

```
fix 1 ellipsoid rigid/meso single
fix 1 rods      rigid/meso molecule
fix 1 spheres   rigid/meso single force 1 off off on
fix 1 particles rigid/meso molecule force 1*5 off off off force 6*10 off off␣
↪on
fix 2 spheres   rigid/meso group 3 sphere1 sphere2 sphere3 torque * off off␣
↪off
```

16.209.3 Description

Treat one or more sets of mesoscopic SPH/SDPD particles as independent rigid bodies. This means that each timestep the total force and torque on each rigid body is computed as the sum of the forces and torques on its constituent particles. The coordinates and velocities of the particles in each body are then updated so that the body moves and rotates as a single entity using the methods described in the paper by *(Miller)*. Density and internal energy of the particles will also be updated. This is implemented by creating internal data structures for each rigid body and performing time integration on these data structures. Positions and velocities of the constituent particles are regenerated from the rigid body data structures in every time step. This restricts which operations and fixes can be applied to rigid bodies. See below for a detailed discussion.

The operation of this fix is exactly like that described by the *fix rigid/nve* command, except that particles' density, internal energy and extrapolated velocity are also updated.

Note: You should not update the particles in rigid bodies via other time-integration fixes (e.g. *fix meso*, *fix meso/stationary*), or you will have conflicting updates to positions and velocities resulting in unphysical behavior in most cases. When performing a hybrid simulation with some atoms in rigid bodies, and some not, a separate time integration fix like *fix meso* should be used for the non-rigid particles.

Note: These fixes are overkill if you simply want to hold a collection of particles stationary or have them move with a constant velocity. To hold particles stationary use *fix meso/stationary* instead. If you would like to move particles with a constant velocity use *fix meso/move*.

Warning: The aggregate properties of each rigid body are calculated at the start of a simulation run and are maintained in internal data structures. The properties include the position and velocity of the center-of-mass of

the body, its moments of inertia, and its angular momentum. This is done using the properties of the constituent particles of the body at that point in time (or see the *infile* keyword option). Thereafter, changing these properties of individual particles in the body will have no effect on a rigid body's dynamics, unless they effect any computation of per-particle forces or torques. If the keyword *reinit* is set to *yes* (the default), the rigid body data structures will be recreated at the beginning of each *run* command; if the keyword *reinit* is set to *no*, the rigid body data structures will be built only at the very first *run* command and maintained for as long as the rigid fix is defined. For example, you might think you could displace the particles in a body or add a large velocity to each particle in a body to make it move in a desired direction before a 2nd run is performed, using the *set* or *displace_atoms* or *velocity* commands. But these commands will not affect the internal attributes of the body unless *reinit* is set to *yes*. With *reinit* set to *no* (or using the *infile* option, which implies *reinit no*) the position and velocity of individual particles in the body will be reset when time integration starts again.

Each rigid body must have two or more particles. A particle can belong to at most one rigid body. Which particles are in which bodies can be defined via several options.

For bodystyle *single* the entire fix group of particles is treated as one rigid body.

For bodystyle *molecule*, particles are grouped into rigid bodies by their respective molecule IDs: each set of particles in the fix group with the same molecule ID is treated as a different rigid body. Note that particles with a molecule ID = 0 will be treated as a single rigid body. For a system with solvent (typically this is particles with molecule ID = 0) surrounding rigid bodies, this may not be what you want. Thus you should be careful to use a fix group that only includes particles you want to be part of rigid bodies.

Bodystyle *custom* is similar to bodystyle *molecule* except that it is more flexible in using other per-atom properties to define the sets of particles that form rigid bodies. An integer vector defined by the *fix property/atom* command can be used. Or an *atom-style or atomfile-style variable* can be used; the floating-point value produced by the variable is rounded to an integer. As with bodystyle *molecule*, each set of particles in the fix groups with the same integer value is treated as a different rigid body. Since fix property/atom vectors and atom-style variables produce values for all particles, you should be careful to use a fix group that only includes particles you want to be part of rigid bodies.

For bodystyle *group*, each of the listed groups is treated as a separate rigid body. Only particles that are also in the fix group are included in each rigid body.

Note: To compute the initial center-of-mass position and other properties of each rigid body, the image flags for each particle in the body are used to "unwrap" the particle coordinates. Thus you must insure that these image flags are consistent so that the unwrapping creates a valid rigid body (one where the particles are close together) , particularly if the particles in a single rigid body straddle a periodic boundary. This means the input data file or restart file must define the image flags for each particle consistently or that you have used the *set* command to specify them correctly. If a dimension is non-periodic then the image flag of each particle must be 0 in that dimension, else an error is generated.

By default, each rigid body is acted on by other particles which induce an external force and torque on its center of mass, causing it to translate and rotate. Components of the external center-of-mass force and torque can be turned off by the *force* and *torque* keywords. This may be useful if you wish a body to rotate but not translate, or vice versa, or if you wish it to rotate or translate continuously unaffected by interactions with other particles. Note that if you expect a rigid body not to move or rotate by using these keywords, you must insure its initial center-of-mass translational or angular velocity is 0.0. Otherwise the initial translational or angular momentum, the body has, will persist.

An xflag, yflag, or zflag set to *off* means turn off the component of force or torque in that dimension. A setting of *on* means turn on the component, which is the default. Which rigid body(s) the settings apply to is determined by the first argument of the *force* and *torque* keywords. It can be an integer M from 1 to Nbody, where Nbody is the number of rigid bodies defined. A wild-card asterisk can be used in place of, or in conjunction with, the M argument to set the flags for multiple rigid bodies. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of rigid bodies, then an asterisk with no numeric values means all bodies from 1 to N. A leading asterisk means all bodies from 1 to n

(inclusive). A trailing asterisk means all bodies from n to N (inclusive). A middle asterisk means all bodies from m to n (inclusive). Note that you can use the *force* or *torque* keywords as many times as you like. If a particular rigid body has its component flags set multiple times, the settings from the final keyword are used.

For computational efficiency, you should typically define one fix rigid/meso command which includes all the desired rigid bodies. LAMMPS will allow multiple rigid/meso fixes to be defined, but it is more expensive.

The keyword/value option pairs are used in the following ways.

The *reinit* keyword determines, whether the rigid body properties are re-initialized between run commands. With the option *yes* (the default) this is done, with the option *no* this is not done. Turning off the re-initialization can be helpful to protect rigid bodies against unphysical manipulations between runs or when properties cannot be easily re-computed (e.g. when read from a file). When using the *infile* keyword, the *reinit* option is automatically set to *no*.

The *infile* keyword allows a file of rigid body attributes to be read in from a file, rather then having LAMMPS compute them. There are 5 such attributes: the total mass of the rigid body, its center-of-mass position, its 6 moments of inertia, its center-of-mass velocity, and the 3 image flags of the center-of-mass position. For rigid bodies consisting of point particles or non-overlapping finite-size particles, LAMMPS can compute these values accurately. However, for rigid bodies consisting of finite-size particles which overlap each other, LAMMPS will ignore the overlaps when computing these 4 attributes. The amount of error this induces depends on the amount of overlap. To avoid this issue, the values can be pre-computed (e.g. using Monte Carlo integration).

The format of the file is as follows. Note that the file does not have to list attributes for every rigid body integrated by fix rigid. Only bodies which the file specifies will have their computed attributes overridden. The file can contain initial blank lines or comment lines starting with "#" which are ignored. The first non-blank, non-comment line should list N = the number of lines to follow. The N successive lines contain the following information:

```
ID1 masstotal xcm ycm zcm ixx iyy izz ixy ixz iyz vxcm vycm vzcm lx ly lz ixcm iycm␣
↪izcm
ID2 masstotal xcm ycm zcm ixx iyy izz ixy ixz iyz vxcm vycm vzcm lx ly lz ixcm iycm␣
↪izcm
...
IDN masstotal xcm ycm zcm ixx iyy izz ixy ixz iyz vxcm vycm vzcm lx ly lz ixcm iycm␣
↪izcm
```

The rigid body IDs are all positive integers. For the *single* bodystyle, only an ID of 1 can be used. For the *group* bodystyle, IDs from 1 to Ng can be used where Ng is the number of specified groups. For the *molecule* bodystyle, use the molecule ID for the atoms in a specific rigid body as the rigid body ID.

The masstotal and center-of-mass coordinates (xcm,ycm,zcm) are self-explanatory. The center-of-mass should be consistent with what is calculated for the position of the rigid body with all its atoms unwrapped by their respective image flags. If this produces a center-of-mass that is outside the simulation box, LAMMPS wraps it back into the box.

The 6 moments of inertia (ixx,iyy,izz,ixy,ixz,iyz) should be the values consistent with the current orientation of the rigid body around its center of mass. The values are with respect to the simulation box XYZ axes, not with respect to the principal axes of the rigid body itself. LAMMPS performs the latter calculation internally.

The (vxcm,vycm,vzcm) values are the velocity of the center of mass. The (lx,ly,lz) values are the angular momentum of the body. The (vxcm,vycm,vzcm) and (lx,ly,lz) values can simply be set to 0 if you wish the body to have no initial motion.

The (ixcm,iycm,izcm) values are the image flags of the center of mass of the body. For periodic dimensions, they specify which image of the simulation box the body is considered to be in. An image of 0 means it is inside the box as defined. A value of 2 means add 2 box lengths to get the true value. A value of -1 means subtract 1 box length to get the true value. LAMMPS updates these flags as the rigid bodies cross periodic boundaries during the simulation.

Note: If you use the *infile* keyword and write restart files during a simulation, then each time a restart file is written, the fix also write an auxiliary restart file with the name rfile.rigid, where "rfile" is the name of the restart file, e.g. tmp.restart.10000 and tmp.restart.10000.rigid. This auxiliary file is in the same format described above. Thus it can be used in a new input script that restarts the run and re-specifies a rigid fix using an *infile* keyword and the appropriate filename. Note that the auxiliary file will contain one line for every rigid body, even if the original file only listed a subset of the rigid bodies.

Restart, fix_modify, output, run start/stop, minimize info:

No information is written to *binary restart files*. If the *infile* keyword is used, an auxiliary file is written out with rigid body information each time a restart file is written, as explained above for the *infile* keyword.

None of the *fix_modify* options are relevant to this fix.

This fix computes a global array of values which can be accessed by various *output commands*.

The number of rows in the array is equal to the number of rigid bodies. The number of columns is 28. Thus for each rigid body, 28 values are stored: the xyz coords of the center of mass (COM), the xyz components of the COM velocity, the xyz components of the force acting on the COM, the components of the 4-vector quaternion representing the orientation of the rigid body, the xyz components of the angular velocity of the body around its COM, the xyz components of the torque acting on the COM, the 3 principal components of the moment of inertia, the xyz components of the angular momentum of the body around its COM, and the xyz image flags of the COM.

The center of mass (COM) for each body is similar to unwrapped coordinates written to a dump file. It will always be inside (or slightly outside) the simulation box. The image flags have the same meaning as image flags for particle positions (see the "dump" command). This means you can calculate the unwrapped COM by applying the image flags to the COM, the same as when unwrapped coordinates are written to a dump file.

The force and torque values in the array are not affected by the *force* and *torque* keywords in the fix rigid command; they reflect values before any changes are made by those keywords.

The ordering of the rigid bodies (by row in the array) is as follows. For the *single* keyword there is just one rigid body. For the *molecule* keyword, the bodies are ordered by ascending molecule ID. For the *group* keyword, the list of group IDs determines the ordering of bodies.

The array values calculated by this fix are "intensive", meaning they are independent of the number of particles in the simulation.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

This fix is not invoked during *energy minimization*.

16.209.4 Restrictions

This fix is part of the USER-SDPD package and also depends on the RIGID package. It is only enabled if LAMMPS was built with both packages. See the *Build package* doc page for more info.

This fix requires that atoms store density and internal energy as defined by the *atom_style meso* command.

All particles in the group must be mesoscopic SPH/SDPD particles.

16.209.5 Related commands

fix meso/move, *fix rigid*, *neigh_modify exclude*

16.209.6 Default

The option defaults are force * on on on and torque * on on on, meaning all rigid bodies are acted on by center-of-mass force and torque. Also reinit = yes.

(Miller) Miller, Eleftheriou, Pattnaik, Ndirango, and Newns, J Chem Phys, 116, 8649 (2002).

16.210 fix rx command

16.211 fix rx/kk command

16.211.1 Syntax

```
fix ID group-ID rx file localTemp matrix solver minSteps ...
```

- ID, group-ID are documented in *fix* command
- rx = style name of this fix command
- file = filename containing the reaction kinetic equations and Arrhenius parameters
- localTemp = *none,lucy* = no local temperature averaging or local temperature defined through Lucy weighting function
- matrix = *sparse, dense* format for the stoichiometric matrix
- solver = *lammps_rk4,rkf45* = rk4 is an explicit 4th order Runge-Kutta method; rkf45 is an adaptive 4th-order Runge-Kutta-Fehlberg method
- minSteps = # of steps for rk4 solver or minimum # of steps for rkf45 (rk4 or rkf45)
- maxSteps = maximum number of steps for the rkf45 solver (rkf45 only)
- relTol = relative tolerance for the rkf45 solver (rkf45 only)
- absTol = absolute tolerance for the rkf45 solver (rkf45 only)
- diag = Diagnostics frequency for the rkf45 solver (optional, rkf45 only)

16.211.2 Examples

```
fix 1 all rx kinetics.rx none dense lammps_rk4
fix 1 all rx kinetics.rx none sparse lammps_rk4 1
fix 1 all rx kinetics.rx lucy sparse lammps_rk4 10
fix 1 all rx kinetics.rx none dense rkf45 1 100 1e-6 1e-8
fix 1 all rx kinetics.rx none dense rkf45 1 100 1e-6 1e-8 -1
```

16.211.3 Description

Fix *rx* solves the reaction kinetic ODEs for a given reaction set that is defined within the file associated with this command.

For a general reaction such that

$$\nu_A A + \nu_B B \rightarrow \nu_C C$$

the reaction rate equation is defined to be of the form

$$r = k(T)[A]^{\nu_A}[B]^{\nu_B}$$

In the current implementation, the exponents are defined to be equal to the stoichiometric coefficients. A given reaction set consisting of *n* reaction equations will contain a total of *m* species. A set of *m* ordinary differential equations (ODEs) that describe the change in concentration of a given species as a function of time are then constructed based on the *n* reaction rate equations.

The ODE systems are solved over the full DPD timestep *dt* using either a 4th order Runge-Kutta *rk4* method with a fixed step-size *h*, specified by the *lammps_rk4* keyword, or a 4th order Runge-Kutta-Fehlberg (rkf45) method with an adaptive step-size for *h*. The number of ODE steps per DPD timestep for the rk4 method is optionally specified immediately after the rk4 keyword. The ODE step-size is set as *dt/num_steps*. Smaller step-sizes tend to yield more accurate results but there is not control on the error. For error control, use the rkf45 ODE solver.

The rkf45 method adjusts the step-size so that the local truncation error is held within the specified absolute and relative tolerances. The initial step-size *h0* can be specified by the user or estimated internally. It is recommended that the user specify *h0* since this will generally reduced the number of ODE integration steps required. *h0* is defined as *dt / min_steps* if min_steps >= 1. If min_steps == 0, *h0* is estimated such that an explicit Euler method would likely produce an acceptable solution. This is generally overly conservative for the 4th-order method and users are advised to specify *h0* as some fraction of the DPD timestep. For small DPD timesteps, only one step may be necessary depending upon the tolerances. Note that more than min_steps ODE steps may be taken depending upon the ODE stiffness but no more than max_steps will be taken. If max_steps is reached, an error warning is printed and the simulation is stopped.

After each ODE step, the solution error *e* is tested and weighted using the absTol and relTol values. The error vector is weighted as *e* / (relTol * |*u*| + absTol) where *u* is the solution vector. If the norm of the error is <= 1, the solution is accepted, *h* is increased by a proportional amount, and the next ODE step is begun. Otherwise, *h* is shrunk and the ODE step is repeated.

Run-time diagnostics are available for the rkf45 ODE solver. The frequency (in time-steps) that diagnostics are reported is controlled by the last (optional) 12th argument. A negative frequency means that diagnostics are reported once at the end of each run. A positive value N means that the diagnostics are reported once per N time-steps.

The diagnostics report the average # of integrator steps and RHS function evaluations and run-time per ODE as well as the average/RMS/min/max per process. If the reporting frequency is 1, the RMS/min/max per ODE are also reported. The per ODE statistics can be used to adjust the tolerance and min/max step parameters. The statistics per MPI process can be useful to examine any load imbalance caused by the adaptive ODE solver. (Some DPD particles can take longer to solve than others. This can lead to an imbalance across the MPI processes.)

The filename specifies a file that contains the entire set of reaction kinetic equations and corresponding Arrhenius parameters. The format of this file is described below.

There is no restriction on the total number or reaction equations that are specified. The species names are arbitrary string names that are associated with the species concentrations. Each species in a given reaction must be preceded by it's stoichiometric coefficient. The only delimiters that are recognized between the species are either a + or = character. The = character corresponds to an irreversible reaction. After specifying the reaction, the reaction rate constant is determined through the temperature dependent Arrhenius equation:

$$k = AT^n e^{\frac{-E_a}{k_B T}}$$

where A is the Arrhenius factor in time units or concentration/time units, n is the unitless exponent of the temperature dependence, and E_a is the activation energy in energy units. The temperature dependence can be removed by specifying the exponent as zero.

The internal temperature of the coarse-grained particles can be used in constructing the reaction rate constants at every DPD timestep by specifying the keyword *none*. Alternatively, the keyword *lucy* can be specified to compute a local-average particle internal temperature for use in the reaction rate constant expressions. The local-average particle internal temperature is defined as:

$$\theta_i^{-1} = \frac{\sum_{j=1} \omega_{Lucy}\left(r_{ij}\right) \theta_j^{-1}}{\sum_{j=1} \omega_{Lucy}\left(r_{ij}\right)}$$

where the Lucy function is expressed as:

$$\omega_{Lucy}\left(r_{ij}\right) = \left(1 + \frac{3r_{ij}}{r_c}\right)\left(1 - \frac{r_{ij}}{r_c}\right)^3$$

The self-particle interaction is included in the above equation.

The stoichiometric coefficients for the reaction mechanism are stored in either a sparse or dense matrix format. The dense matrix should only be used for small reaction mechanisms. The sparse matrix should be used when there are many reactions (e.g., more than 5). This allows the number of reactions and species to grow while keeping the computational cost tractable. The matrix format can be specified as using either the *sparse* or *dense* keywords. If all stoichiometric coefficients for a reaction are small integers (whole numbers <= 3), a fast exponential function is used. This can save significant computational time so users are encouraged to use integer coefficients where possible.

The format of a tabulated file is as follows (without the parenthesized comments):

```
# Rxn equations and parameters                                          (one or␣
↪more comment or blank lines)

1.0 hcn + 1.0 no2 = 1.0  no + 0.5 n2  + 0.5 h2 + 1.0 co   2.49E+01 0.0 1.34  (rxn␣
↪equation, A, n, Ea)
1.0 hcn + 1.0  no = 1.0  co + 1.0 n2  + 0.5 h2            2.16E+00 0.0 1.52
...
1.0  no + 1.0  co = 0.5  n2 + 1.0 co2                     1.66E+06 0.0 0.69
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections.

Following a blank line, the next N lines list the N reaction equations. Each species within the reaction equation is specified through its stoichiometric coefficient and a species tag. Reactant species are specified on the left-hand side of the equation and product species are specified on the right-hand side of the equation. After specifying the reactant and product species, the final three arguments of each line represent the Arrhenius parameter A, the temperature exponent n, and the activation energy Ea.

Note that the species tags that are defined in the reaction equations are used by the *fix eos/table/rx* command to define the thermodynamic properties of each species. Furthermore, the number of species molecules (i.e., concentration) can be specified either with the *set* command using the "d_" prefix or by reading directly the concentrations from a data file. For the latter case, the *read_data* command with the fix keyword should be specified, where the fix-ID will be the "fix rx`ID with a <SPECIES">`_ suffix, e.g.

fix foo all rx reaction.file … read_data data.dpd fix foo_SPECIES NULL Species

---

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages*

doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

16.211.4 Restrictions

This command is part of the USER-DPD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This command also requires use of the *atom_style dpd* command.

This command can only be used with a constant energy or constant enthalpy DPD simulation.

16.211.5 Related commands

fix eos/table/rx, *fix shardlow*, *pair dpd/fdt/energy*

Default: none

16.212 fix saed/vtk command

16.212.1 Syntax

```
fix ID group-ID saed/vtk Nevery Nrepeat Nfreak c_ID attribute args ... keyword args ..
↪.
```

- ID, group-ID are documented in *fix* command
- saed/vtk = style name of this fix command
- Nevery = use input values every this many timesteps
- Nrepeat = # of times to use input values for calculating averages
- Nfreq = calculate averages every this many timesteps
- c_ID = saed compute ID

```
keyword = file or ave or start or file or overwrite:l
  ave args = one or running or window M
    one = output a new average value every Nfreq steps
    running = output cumulative average of all previous Nfreq steps
    window M = output average of M most recent Nfreq steps
  start args = Nstart
    Nstart = start averaging on this timestep
  file arg = filename
    filename = name of file to output time averages to
  overwrite arg = none = overwrite output file with only latest output
```

16.212.2 Examples

```
compute 1 all saed 0.0251 Al O Kmax 1.70 Zone 0 0 1 dR_Ewald 0.01 c 0.5 0.5 0.5
compute 2 all saed 0.0251 Ni Kmax 1.70 Zone 0 0 0 c 0.05 0.05 0.05 manual echo

fix 1 all saed/vtk 1 1 1 c_1 file Al2O3_001.saed
fix 2 all saed/vtk 1 1 1 c_2 file Ni_000.saed
```

16.212.3 Description

Time average computed intensities from *compute saed* and write output to a file in the 3rd generation vtk image data format for visualization directly in parallelized visualization software packages like ParaView and VisIt. Note that if no time averaging is done, this command can be used as a convenient way to simply output diffraction intensities at a single snapshot.

To produce output in the image data vtk format ghost data is added outside the *Kmax* range assigned in the compute saed. The ghost data is assigned a value of -1 and can be removed setting a minimum isovolume of 0 within the visualization software. SAED images can be created by visualizing a spherical slice of the data that is centered at R_Ewald*[h k l]/norm([h k l]), where R_Ewald=1/lambda.

The group specified within this command is ignored. However, note that specified values may represent calculations performed by saed computes which store their own "group" definitions.

Fix saed/vtk is designed to work only with *compute saed* values, e.g.

```
compute 3 top saed 0.0251 Al O
fix saed/vtk 1 1 1 c_3 file Al2O3_001.saed
```

The *Nevery*, *Nrepeat*, and *Nfreq* arguments specify on what timesteps the input values will be used in order to contribute to the average. The final averaged quantities are generated on timesteps that are a multiple of *Nfreq*. The average is over *Nrepeat* quantities, computed in the preceding portion of the simulation every *Nevery* timesteps. *Nfreq* must be a multiple of *Nevery* and *Nevery* must be non-zero even if *Nrepeat* is 1. Also, the timesteps contributing to the average value cannot overlap, i.e. Nrepeat*Nevery can not exceed Nfreq.

For example, if Nevery=2, Nrepeat=6, and Nfreq=100, then values on timesteps 90,92,94,96,98,100 will be used to compute the final average on timestep 100. Similarly for timesteps 190,192,194,196,198,200 on timestep 200, etc. If Nrepeat=1 and Nfreq = 100, then no time averaging is done; values are simply generated on timesteps 100,200,etc.

The output for fix ave/time/saed is a file written with the 3rd generation vtk image data formatting. The filename assigned by the *file* keyword is appended with _N.vtk where N is an index (0,1,2...) to account for multiple diffraction intensity outputs.

By default the header contains the following information (with example data):

```
# vtk DataFile Version 3.0 c_SAED
Image data set
ASCII
DATASET STRUCTURED_POINTS
DIMENSIONS 337 219 209
ASPECT_RATIO 0.00507953 0.00785161 0.00821458
ORIGIN -0.853361 -0.855826 -0.854316
POINT_DATA 15424827
SCALARS intensity float
```

(continues on next page)

(continued from previous page)

```
LOOKUP_TABLE default
...data
```

In this example, kspace is sampled across a 337 x 219 x 209 point mesh where the mesh spacing is approximately 0.005, 0.007, and 0.008 inv(length) units in the k1, k2, and k3 directions, respectively. The data is shifted by -0.85, -0.85, -0.85 inv(length) units so that the origin will lie at 0, 0, 0. Here, 15,424,827 kspace points are sampled in total.

Additional optional keywords also affect the operation of this fix.

The *ave* keyword determines how the values produced every *Nfreq* steps are averaged with values produced on previous steps that were multiples of *Nfreq*, before they are accessed by another output command or written to a file.

If the *ave* setting is *one*, then the values produced on timesteps that are multiples of *Nfreq* are independent of each other; they are output as-is without further averaging.

If the *ave* setting is *running*, then the values produced on timesteps that are multiples of *Nfreq* are summed and averaged in a cumulative sense before being output. Each output value is thus the average of the value produced on that timestep with all preceding values. This running average begins when the fix is defined; it can only be restarted by deleting the fix via the *unfix* command, or by re-defining the fix by re-specifying it.

If the *ave* setting is *window*, then the values produced on timesteps that are multiples of *Nfreq* are summed and averaged within a moving "window" of time, so that the last M values are used to produce the output. E.g. if M = 3 and Nfreq = 1000, then the output on step 10000 will be the average of the individual values on steps 8000,9000,10000. Outputs on early steps will average over less than M values if they are not available.

The *start* keyword specifies what timestep averaging will begin on. The default is step 0. Often input values can be 0.0 at time 0, so setting *start* to a larger value can avoid including a 0.0 in a running or windowed average.

The *file* keyword allows a filename to be specified. Every *Nfreq* steps, the vector of saed intensity data is written to a new file using the 3rd generation vtk format. The base of each file is assigned by the *file* keyword and this string is appended with _N.vtk where N is an index (0,1,2...) to account for situations with multiple diffraction intensity outputs.

The *overwrite* keyword will continuously overwrite the output file with the latest output, so that it only contains one timestep worth of output. This option can only be used with the *ave running* setting.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.212.4 Restrictions

The attributes for fix_saed_vtk must match the values assigned in the associated *compute_saed* command.

16.212.5 Related commands

compute_saed

16.212.6 Default

The option defaults are ave = one, start = 0, no file output.

(Coleman) Coleman, Spearot, Capolungo, MSMSE, 21, 055020 (2013).

16.213 fix setforce command

16.214 fix setforce/kk command

16.215 fix setforce/spin command

16.215.1 Syntax

```
fix ID group-ID setforce fx fy fz keyword value ...
```

- ID, group-ID are documented in *fix* command
- setforce = style name of this fix command
- fx,fy,fz = force component values
- any of fx,fy,fz can be a variable (see below)
- zero or more keyword/value pairs may be appended to args
- keyword = *region*

  ```
  region value = region-ID
    region-ID = ID of region atoms must be in to have added force
  ```

16.215.2 Examples

```
fix freeze indenter setforce 0.0 0.0 0.0
fix 2 edge setforce NULL 0.0 0.0
fix 1 edge setforce/spin 0.0 0.0 0.0
fix 2 edge setforce NULL 0.0 v_oscillate
```

16.215.3 Description

Set each component of force on each atom in the group to the specified values fx,fy,fz. This erases all previously computed forces on the atom, though additional fixes could add new forces. This command can be used to freeze certain atoms in the simulation by zeroing their force, either for running dynamics or performing an energy minimization. For dynamics, this assumes their initial velocity is also zero.

Any of the fx,fy,fz values can be specified as NULL which means do not alter the force component in that dimension.

Any of the 3 quantities defining the force components can be specified as an equal-style or atom-style *variable*, namely *fx*, *fy*, *fz*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the force component.

Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent force field.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent force field with optional time-dependence as well.

If the *region* keyword is used, the atom must also be in the specified geometric *region* in order to have force added to it.

Style *spin* suffix sets the components of the magnetic precession vectors instead of the mechanical forces. This also erases all previously computed magnetic precession vectors on the atom, though additional magnetic fixes could add new forces.

This command can be used to freeze the magnetic moment of certain atoms in the simulation by zeroing their precession vector.

All options defined above remain valid, they just apply to the magnetic precession vectors instead of the forces.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

The region keyword is also supported by Kokkos, but a Kokkos-enabled region must be used. See the region *region* command for more information.

These accelerated styles are part of the r Kokkos package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix is setting the forces to the desired values; on all other levels, the force is set to 0.0 for the atoms in the fix group, so that setforce values are not counted multiple times. Default is to to override forces at the outermost level.

This fix computes a global 3-vector of forces, which can be accessed by various *output commands*. This is the total force on the group of atoms before the forces on individual atoms are changed by the fix. The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command, but you cannot set forces to any value besides zero when performing a minimization. Use the *fix addforce* command if you want to apply a non-zero force to atoms during a minimization.

16.215.4 Restrictions

The fix *setforce/spin* only makes sense when LAMMPS was built with the SPIN package.

16.215.5 Related commands

fix addforce, *fix aveforce*

Default: none

16.216 fix shake command

16.217 fix rattle command

16.217.1 Syntax

```
fix ID group-ID style tol iter N constraint values ... keyword value ...
```

- ID, group-ID are documented in *fix* command
- style = shake or rattle = style name of this fix command
- tol = accuracy tolerance of SHAKE solution
- iter = max # of iterations in each SHAKE solution
- N = print SHAKE statistics every this many timesteps (0 = never)
- one or more constraint/value pairs are appended
- constraint = *b* or *a* or *t* or *m*

```
b values = one or more bond types
a values = one or more angle types
t values = one or more atom types
m value = one or more mass values
```

- zero or more keyword/value pairs may be appended
- keyword = *mol*

```
mol value = template-ID
  template-ID = ID of molecule template specified in a separate molecule␣
↪command
```

16.217.2 Examples

```
fix 1 sub shake 0.0001 20 10 b 4 19 a 3 5 2
fix 1 sub shake 0.0001 20 10 t 5 6 m 1.0 a 31
fix 1 sub shake 0.0001 20 10 t 5 6 m 1.0 a 31 mol myMol
fix 1 sub rattle 0.0001 20 10 t 5 6 m 1.0 a 31
fix 1 sub rattle 0.0001 20 10 t 5 6 m 1.0 a 31 mol myMol
```

16.217.3 Description

Apply bond and angle constraints to specified bonds and angles in the simulation by either the SHAKE or RATTLE algorithms. This typically enables a longer timestep.

SHAKE vs RATTLE:

The SHAKE algorithm was invented for schemes such as standard Verlet timestepping, where only the coordinates are integrated and the velocities are approximated as finite differences to the trajectories (*Ryckaert et al. (1977)*). If the velocities are integrated explicitly, as with velocity Verlet which is what LAMMPS uses as an integration method, a second set of constraining forces is required in order to eliminate velocity components along the bonds (*Andersen (1983)*).

In order to formulate individual constraints for SHAKE and RATTLE, focus on a single molecule whose bonds are constrained. Let Ri and Vi be the position and velocity of atom *i* at time *n*, for *i* =1,. . . ,*N*, where *N* is the number of sites of our reference molecule. The distance vector between sites *i* and *j* is given by

$$\mathbf{r}_{ij}^{n+1} = \mathbf{r}_j^n - \mathbf{r}_i^n$$

The constraints can then be formulated as

$$\mathbf{r}_{ij}^{n+1} \cdot \mathbf{r}_{ij}^{n+1} = d_{ij}^2 \quad \text{and}$$
$$\mathbf{v}_{ij}^{n+1} \cdot \mathbf{r}_{ij}^{n+1} = 0$$

The SHAKE algorithm satisfies the first condition, i.e. the sites at time *n+1* will have the desired separations Dij immediately after the coordinates are integrated. If we also enforce the second condition, the velocity components along the bonds will vanish. RATTLE satisfies both conditions. As implemented in LAMMPS, fix rattle uses fix shake for satisfying the coordinate constraints. Therefore the settings and optional keywords are the same for both fixes, and all the information below about SHAKE is also relevant for RATTLE.

SHAKE:

Each timestep the specified bonds and angles are reset to their equilibrium lengths and angular values via the SHAKE algorithm (*Ryckaert et al. (1977)*). This is done by applying an additional constraint force so that the new positions preserve the desired atom separations. The equations for the additional force are solved via an iterative method that typically converges to an accurate solution in a few iterations. The desired tolerance (e.g. 1.0e-4 = 1 part in 10000) and maximum # of iterations are specified as arguments. Setting the N argument will print statistics to the screen and log file about regarding the lengths of bonds and angles that are being constrained. Small delta values mean SHAKE is doing a good job.

In LAMMPS, only small clusters of atoms can be constrained. This is so the constraint calculation for a cluster can be performed by a single processor, to enable good parallel performance. A cluster is defined as a central atom connected to others in the cluster by constrained bonds. LAMMPS allows for the following kinds of clusters to be constrained: one central atom bonded to 1 or 2 or 3 atoms, or one central atom bonded to 2 others and the angle between the 3 atoms also constrained. This means water molecules or CH2 or CH3 groups may be constrained, but not all the C-C backbone bonds of a long polymer chain.

The *b* constraint lists bond types that will be constrained. The *t* constraint lists atom types. All bonds connected to an atom of the specified type will be constrained. The *m* constraint lists atom masses. All bonds connected to atoms

of the specified masses will be constrained (within a fudge factor of MASSDELTA specified in fix_shake.cpp). The *a* constraint lists angle types. If both bonds in the angle are constrained then the angle will also be constrained if its type is in the list.

For all constraints, a particular bond is only constrained if both atoms in the bond are in the group specified with the SHAKE fix.

The degrees-of-freedom removed by SHAKE bonds and angles are accounted for in temperature and pressure computations. Similarly, the SHAKE contribution to the pressure of the system (virial) is also accounted for.

Note: This command works by using the current forces on atoms to calculate an additional constraint force which when added will leave the atoms in positions that satisfy the SHAKE constraints (e.g. bond length) after the next time integration step. If you define fixes (e.g. *fix efield*) that add additional force to the atoms after fix shake operates, then this fix will not take them into account and the time integration will typically not satisfy the SHAKE constraints. The solution for this is to make sure that fix shake is defined in your input script after any other fixes which add or change forces (to atoms that fix shake operates on).

The *mol* keyword should be used when other commands, such as *fix deposit* or *fix pour*, add molecules on-the-fly during a simulation, and you wish to constrain the new molecules via SHAKE. You specify a *template-ID* previously defined using the *molecule* command, which reads a file that defines the molecule. You must use the same *template-ID* that the command adding molecules uses. The coordinates, atom types, special bond restrictions, and SHAKE info can be specified in the molecule file. See the *molecule* command for details. The only settings required to be in this file (by this command) are the SHAKE info of atoms in the molecule.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

RATTLE:

The velocity constraints lead to a linear system of equations which can be solved analytically. The implementation of the algorithm in LAMMPS closely follows (*Andersen (1983)*).

Note: The fix rattle command modifies forces and velocities and thus should be defined after all other integration fixes in your input script. If you define other fixes that modify velocities or forces after fix rattle operates, then fix rattle will not take them into account and the overall time integration will typically not satisfy the RATTLE constraints. You can check whether the constraints work correctly by setting the value of RATTLE_DEBUG in src/fix_rattle.cpp to 1 and recompiling LAMMPS.

Restart, fix_modify, output, run start/stop, minimize info:

The *fix_modify virial* option is supported by this fix to add the contribution due to keeping the constraints to the system's virial as part of *thermodynamic output*. The default is *virial yes*

No information about these fixes is written to *binary restart files*. None of the *fix_modify* options are relevant to these fixes. No global or per-atom quantities are stored by these fixes for access by various *output commands*. No parameter of these fixes can be used with the *start/stop* keywords of the *run* command. These fixes are not invoked during *energy minimization*.

16.217.4 Restrictions

These fixes are part of the RIGID package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

For computational efficiency, there can only be one shake or rattle fix defined in a simulation.

If you use a tolerance that is too large or a max-iteration count that is too small, the constraints will not be enforced very strongly, which can lead to poor energy conservation. You can test for this in your system by running a constant NVE simulation with a particular set of SHAKE parameters and monitoring the energy versus time.

SHAKE or RATTLE should not be used to constrain an angle at 180 degrees (e.g. linear CO2 molecule). This causes numeric difficulties. You can use *fix rigid or fix rigid/small* instead to make a linear molecule rigid.

Related commands: none

Default: none

(Ryckaert) J.-P. Ryckaert, G. Ciccotti and H. J. C. Berendsen, J of Comp Phys, 23, 327-341 (1977).

(Andersen) H. Andersen, J of Comp Phys, 52, 24-34 (1983).

16.218 fix shardlow command

16.219 fix shardlow/kk command

16.219.1 Syntax

```
fix ID group-ID shardlow
```

- ID, group-ID are documented in *fix* command
- shardlow = style name of this fix command

16.219.2 Examples

```
fix 1 all shardlow
```

16.219.3 Description

Specifies that the Shardlow splitting algorithm (SSA) is to be used to integrate the DPD equations of motion. The SSA splits the integration into a stochastic and deterministic integration step. The fix *shardlow* performs the stochastic integration step and must be used in conjunction with a deterministic integrator (e.g. *fix nve* or *fix nph*). The stochastic integration of the dissipative and random forces is performed prior to the deterministic integration of the conservative force. Further details regarding the method are provided in *(Lisal)* and *(Larentzos1)*.

The fix *shardlow* must be used with the *pair_style dpd/fdt* or *pair_style dpd/fdt/energy* command to properly initialize the fluctuation-dissipation theorem parameter(s) sigma (and kappa, if necessary).

Note that numerous variants of DPD can be specified by choosing an appropriate combination of the integrator and *pair_style dpd/fdt* command. DPD under isothermal conditions can be specified by using fix *shardlow*, fix *nve* and pair_style *dpd/fdt*. DPD under isoenergetic conditions can be specified by using fix *shardlow*, fix *nve* and pair_style *dpd/fdt/energy*. DPD under isobaric conditions can be specified by using fix shardlow, fix *nph* and pair_style *dpd/fdt*. DPD under isoenthalpic conditions can be specified by using fix shardlow, fix *nph* and pair_style *dpd/fdt/energy*. Examples of each DPD variant are provided in the examples/USER/dpd directory.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

16.219.4 Restrictions

This command is part of the USER-DPD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix is currently limited to orthogonal simulation cell geometries.

This fix must be used with an additional fix that specifies time integration, e.g. *fix nve* or *fix nph*.

The Shardlow splitting algorithm requires the sizes of the sub-domain lengths to be larger than twice the cutoff+skin. Generally, the domain decomposition is dependent on the number of processors requested.

16.219.5 Related commands

pair_style dpd/fdt, *fix eos/cv*

Default: none

(Lisal) M. Lisal, J.K. Brennan, J. Bonet Avalos, "Dissipative particle dynamics as isothermal, isobaric, isoenergetic, and isoenthalpic conditions using Shardlow-like splitting algorithms.", J. Chem. Phys., 135, 204105 (2011).

(Larentzos1) J.P. Larentzos, J.K. Brennan, J.D. Moore, M. Lisal and W.D. Mattson, "Parallel Implementation of Isothermal and Isoenergetic Dissipative Particle Dynamics Using Shardlow-Like Splitting Algorithms", Comput. Phys. Commun., 185, 1987-1998 (2014).

(Larentzos2) J.P. Larentzos, J.K. Brennan, J.D. Moore, and W.D. Mattson, "LAMMPS Implementation of Constant Energy Dissipative Particle Dynamics (DPD-E)", ARL-TR-6863, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD (2014).

16.220 fix smd command

16.220.1 Syntax

```
fix ID group-ID smd type values keyword values
```

- ID, group-ID are documented in *fix* command
- smd = style name of this fix command
- mode = *cvel* or *cfor* to select constant velocity or constant force SMD

```
cvel values = K vel
  K = spring constant (force/distance units)
  vel = velocity of pulling (distance/time units)
cfor values = force
  force = pulling force (force units)
```

- keyword = *tether* or *couple*

```
tether values = x y z R0
  x,y,z = point to which spring is tethered
  R0 = distance of end of spring from tether point (distance units)
couple values = group-ID2 x y z R0
  group-ID2 = 2nd group to couple to fix group with a spring
  x,y,z = direction of spring, automatically computed with 'auto'
  R0 = distance of end of spring (distance units)
```

16.220.2 Examples

```
fix  pull    cterm smd cvel 20.0 -0.00005 tether NULL NULL 100.0 0.0
fix  pull    cterm smd cvel 20.0 -0.0001 tether 25.0 25 25.0 0.0
fix  stretch cterm smd cvel 20.0  0.0001 couple nterm auto auto auto 0.0
fix  pull    cterm smd cfor  5.0 tether 25.0 25.0 25.0 0.0
```

16.220.3 Description

This fix implements several options of steered MD (SMD) as reviewed in *(Izrailev)*, which allows to induce conformational changes in systems and to compute the potential of mean force (PMF) along the assumed reaction coordinate *(Park)* based on Jarzynski's equality *(Jarzynski)*. This fix borrows a lot from *fix spring* and *fix setforce*.

You can apply a moving spring force to a group of atoms (*tether* style) or between two groups of atoms (*couple* style). The spring can then be used in either constant velocity (*cvel*) mode or in constant force (*cfor*) mode to induce transitions in your systems. When running in *tether* style, you may need some way to fix some other part of the system (e.g. via *fix spring/self*)

The *tether* style attaches a spring between a point at a distance of R0 away from a fixed point *x,y,z* and the center of mass of the fix group of atoms. A restoring force of magnitude K (R - R0) Mi / M is applied to each atom in the group where *K* is the spring constant, Mi is the mass of the atom, and M is the total mass of all atoms in the group. Note that *K* thus represents the total force on the group of atoms, not a per-atom force.

In *cvel* mode the distance R is incremented or decremented monotonously according to the pulling (or pushing) velocity. In *cfor* mode a constant force is added and the actual distance in direction of the spring is recorded.

The *couple* style links two groups of atoms together. The first group is the fix group; the second is specified by group-ID2. The groups are coupled together by a spring that is at equilibrium when the two groups are displaced by a vector in direction *x,y,z* with respect to each other and at a distance R0 from that displacement. Note that *x,y,z* only provides a direction and will be internally normalized. But since it represents the *absolute* displacement of group-ID2 relative to the fix group, (1,1,0) is a different spring than (-1,-1,0). For each vector component, the displacement can be described with the *auto* parameter. In this case the direction is re-computed in every step, which can be useful for steering a local process where the whole object undergoes some other change. When the relative positions and distance between the two groups are not in equilibrium, the same spring force described above is applied to atoms in each of the two groups.

For both the *tether* and *couple* styles, any of the x,y,z values can be specified as NULL which means do not include that dimension in the distance calculation or force application.

For constant velocity pulling (*cvel* mode), the running integral over the pulling force in direction of the spring is recorded and can then later be used to compute the potential of mean force (PMF) by averaging over multiple independent trajectories along the same pulling path.

Restart, fix_modify, output, run start/stop, minimize info:

The fix stores the direction of the spring, current pulling target distance and the running PMF to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify virial* option is supported by this fix to add the contribution due to the added forces on atoms to the system's virial as part of *thermodynamic output*. The default is *virial no*

The *fix_modify respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix is adding its forces. Default is the outermost level.

This fix computes a vector list of 7 quantities, which can be accessed by various *output commands*. The quantities in the vector are in this order: the x-, y-, and z-component of the pulling force, the total force in direction of the pull, the equilibrium distance of the spring, the distance between the two reference points, and finally the accumulated PMF (the sum of pulling forces times displacement).

The force is the total force on the group of atoms by the spring. In the case of the *couple* style, it is the force on the fix group (group-ID) or the negative of the force on the 2nd group (group-ID2). The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.220.4 Restrictions

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.220.5 Related commands

fix drag, *fix spring*, *fix spring/self*, *fix spring/rg*, *fix colvars*, *fix plumed*

Default: none

(Izrailev) Izrailev, Stepaniants, Isralewitz, Kosztin, Lu, Molnar, Wriggers, Schulten. Computational Molecular Dynamics: Challenges, Methods, Ideas, volume 4 of Lecture Notes in Computational Science and Engineering, pp. 39-65. Springer-Verlag, Berlin, 1998.

(Park) Park, Schulten, J. Chem. Phys. 120 (13), 5946 (2004)

(Jarzynski) Jarzynski, Phys. Rev. Lett. 78, 2690 (1997)

16.221 fix smd/adjust_dt command

16.221.1 Syntax

```
fix ID group-ID smd/adjust_dt arg
```

- ID, group-ID are documented in *fix* command
- smd/adjust_dt = style name of this fix command
- arg = *s_fact*

  s_fact = safety factor

16.221.2 Examples

```
fix 1 all smd/adjust_dt 0.1
```

16.221.3 Description

The fix calculates a new stable time increment for use with the SMD time integrators.

The stable time increment is based on multiple conditions. For the SPH pair styles, a CFL criterion (Courant, Friedrichs & Lewy, 1928) is evaluated, which determines the speed of sound cannot propagate further than a typical spacing between particles within a single time step to ensure no information is lost. For the contact pair styles, a linear analysis of the pair potential determines a stable maximum time step.

This fix inquires the minimum stable time increment across all particles contained in the group for which this fix is defined. An additional safety factor *s_fact* is applied to the time increment.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Restart, fix_modify, output, run start/stop, minimize info:

Currently, no part of USER-SMD supports restarting nor minimization.

16.221.4 Restrictions

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.221.5 Related commands

smd/tlsph_dt

Default: none

16.222 fix smd/integrate_tlsph command

16.222.1 Syntax

```
fix ID group-ID smd/integrate_tlsph keyword values
```

- ID, group-ID are documented in *fix* command
- smd/integrate_tlsph = style name of this fix command
- zero or more keyword/value pairs may be appended
- keyword = *limit_velocity*

```
limit_velocity value = max_vel
  max_vel = maximum allowed velocity
```

16.222.2 Examples

```
fix 1 all smd/integrate_tlsph
fix 1 all smd/integrate_tlsph limit_velocity 1000
```

16.222.3 Description

The fix performs explicit time integration for particles which interact according with the Total-Lagrangian SPH pair style.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

The *limit_velocity* keyword will control the velocity, scaling the norm of the velocity vector to max_vel in case it exceeds this velocity limit.

Restart, fix_modify, output, run start/stop, minimize info:

Currently, no part of USER-SMD supports restarting nor minimization. This fix has no outputs.

16.222.4 Restrictions

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.222.5 Related commands

smd/integrate_ulsph

Default: none

16.223 fix smd/integrate_ulsph command

16.223.1 Syntax

```
fix ID group-ID smd/integrate_ulsph keyword
```

- ID, group-ID are documented in *fix* command
- smd/integrate_ulsph = style name of this fix command
- zero or more keyword/value pairs may be appended
- keyword = adjust_radius or limit_velocity

adjust_radius values = adjust_radius_factor min_nn max_nn adjust_radius_factor = factor which scale the smooth/kernel radius min_nn = minimum number of neighbors max_nn = maximum number of neighbors

limit_velocity values = max_velocity max_velocity = maximum allowed velocity.

16.223.2 Examples

```
fix 1 all smd/integrate_ulsph adjust_radius 1.02 25 50
fix 1 all smd/integrate_ulsph limit_velocity 1000
```

16.223.3 Description

The fix performs explicit time integration for particles which interact with the updated Lagrangian SPH pair style.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

The *adjust_radius* keyword activates dynamic adjustment of the per-particle SPH smoothing kernel radius such that the number of neighbors per particles remains within the interval *min_nn* to *max_nn*. The parameter *adjust_radius_factor* determines the amount of adjustment per timestep. Typical values are *adjust_radius_factor* =1.02, *min_nn* =15, and *max_nn* =20.

The *limit_velocity* keyword will control the velocity, scaling the norm of the velocity vector to max_vel in case it exceeds this velocity limit.

Restart, fix_modify, output, run start/stop, minimize info:

Currently, no part of USER-SMD supports restarting nor minimization. This fix has no outputs.

16.223.4 Restrictions

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Related commands: none

Default: none

16.224 fix smd/move_tri_surf command

16.224.1 Syntax

```
fix ID group-ID smd/move_tri_surf keyword
```

- ID, group-ID are documented in *fix* command
- smd/move_tri_surf keyword = style name of this fix command
- keyword = **LINEAR* or **WIGGLE* or **ROTATE*

```
*LINEAR args = Vx Vy Vz
   Vx,Vy,Vz = components of velocity vector (velocity units), any␣
↪component can be specified as NULL
*WIGGLE args = Vx Vy Vz max_travel
   vx,vy,vz = components of velocity vector (velocity units), any␣
↪component can be specified as NULL
   max_travel = wiggle amplitude
*ROTATE args = Px Py Pz Rx Ry Rz period
   Px,Py,Pz = origin point of axis of rotation (distance units)
   Rx,Ry,Rz = axis of rotation vector
   period = period of rotation (time units)
```

16.224.2 Examples

```
fix 1 tool smd/move_tri_surf *LINEAR 20 20 10
fix 2 tool smd/move_tri_surf *WIGGLE 20 20 10
fix 2 tool smd/move_tri_surf *ROTATE 0 0 0 5 2 1
```

16.224.3 Description

This fix applies only to rigid surfaces read from .STL files via fix *smd/wall_surface* . It updates position and velocity for the particles in the group each timestep without regard to forces on the particles. The rigid surfaces can thus be moved along simple trajectories during the simulation.

The **LINEAR* style moves particles with the specified constant velocity vector V = (Vx,Vy,Vz). This style also sets the velocity of each particle to V = (Vx,Vy,Vz).

The **WIGGLE* style moves particles in an oscillatory fashion. Particles are moved along (vx, vy, vz) with constant velocity until a displacement of max_travel is reached. Then, the velocity vector is reversed. This process is repeated.

The **ROTATE* style rotates particles around a rotation axis R = (Rx,Ry,Rz) that goes through a point P = (Px,Py,Pz). The period of the rotation is also specified. This style also sets the velocity of each particle to (omega cross Rperp)

where omega is its angular velocity around the rotation axis and Rperp is a perpendicular vector from the rotation axis to the particle.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Restart, fix_modify, output, run start/stop, minimize info:

Currently, no part of USER-SMD supports restarting nor minimization. This fix has no outputs.

16.224.4 Restrictions

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.224.5 Related commands

smd/triangle_mesh_vertices, *smd/wall_surface*

Default: none

16.225 fix smd/setvel command

16.225.1 Syntax

```
fix ID group-ID smd/setvel vx vy vz keyword value ...
```

- ID, group-ID are documented in *fix* command
- smd/setvel = style name of this fix command
- vx,vy,vz = velocity component values
- any of vx,vy,vz can be a variable (see below)
- zero or more keyword/value pairs may be appended to args
- keyword = *region*

```
region value = region-ID
  region-ID = ID of region particles must be in to have their velocities␣
↪set
```

16.225.2 Examples

```
fix top_velocity top_group setvel 1.0 0.0 0.0
```

16.225.3 Description

Set each component of velocity on each particle in the group to the specified values vx,vy,vz, regardless of the forces acting on the particle. This command can be used to impose velocity boundary conditions.

Any of the vx,vy,vz values can be specified as NULL which means do not alter the velocity component in that dimension.

This fix is indented to be used together with a time integration fix.

Any of the 3 quantities defining the velocity components can be specified as an equal-style or atom-style *variable*, namely *vx*, *vy*, *vz*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the force component.

Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent velocity field.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent velocity field with optional time-dependence as well.

If the *region* keyword is used, the particle must also be in the specified geometric *region* in order to have its velocity set by this command.

Restart, fix_modify, output, run start/stop, minimize info:

Currently, no part of USER-SMD supports restarting nor minimization None of the *fix_modify* options are relevant to this fix.

This fix computes a global 3-vector of forces, which can be accessed by various *output commands*. This is the total force on the group of atoms. The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

16.225.4 Restrictions

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Related commands: none

Default: none

16.226 fix smd/wall_surface command

16.226.1 Syntax

```
fix ID group-ID smd/wall_surface arg type mol-ID
```

- ID, group-ID are documented in *fix* command
- smd/wall_surface = style name of this fix command
- arg = *file*

  file = file name of a triangular mesh in stl format

- type = particle type to be given to the new particles created by this fix
- mol-ID = molecule-ID to be given to the new particles created by this fix (must be >= 65535)

16.226.2 Examples

```
fix stl_surf all smd/wall_surface tool.stl 2 65535
```

16.226.3 Description

This fix creates reads a triangulated surface from a file in .STL format. For each triangle, a new particle is created which stores the barycenter of the triangle and the vertex positions. The radius of the new particle is that of the minimum circle which encompasses the triangle vertices.

The triangulated surface can be used as a complex rigid wall via the *smd/tri_surface* pair style. It is possible to move the triangulated surface via the *smd/move_tri_surf* fix style.

Immediately after a .STL file has been read, the simulation needs to be run for 0 timesteps in order to properly register the new particles in the system. See the "funnel_flow" example in the USER-SMD examples directory.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Restart, fix_modify, output, run start/stop, minimize info:

Currently, no part of USER-SMD supports restarting nor minimization. This fix has no outputs.

16.226.4 Restrictions

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

The molecule ID given to the particles created by this fix have to be equal to or larger than 65535.

Within each .STL file, only a single triangulated object must be present, even though the STL format allows for the possibility of multiple objects in one file.

16.226.5 Related commands

smd/triangle_mesh_vertices, *smd/move_tri_surf*, *smd/tri_surface*

Default: none

16.227 fix spring command

16.227.1 Syntax

```
fix ID group-ID spring keyword values
```

- ID, group-ID are documented in *fix* command
- spring = style name of this fix command
- keyword = *tether* or *couple*

```
tether values = K x y z R0
  K = spring constant (force/distance units)
  x,y,z = point to which spring is tethered
  R0 = equilibrium distance from tether point (distance units)
couple values = group-ID2 K x y z R0
  group-ID2 = 2nd group to couple to fix group with a spring
  K = spring constant (force/distance units)
  x,y,z = direction of spring
  R0 = equilibrium distance of spring (distance units)
```

16.227.2 Examples

```
fix pull ligand spring tether 50.0 0.0 0.0 0.0 0.0
fix pull ligand spring tether 50.0 0.0 0.0 0.0 5.0
fix pull ligand spring tether 50.0 NULL NULL 2.0 3.0
fix 5 bilayer1 spring couple bilayer2 100.0 NULL NULL 10.0 0.0
fix longitudinal pore spring couple ion 100.0 NULL NULL -20.0 0.0
fix radial pore spring couple ion 100.0 0.0 0.0 NULL 5.0
```

16.227.3 Description

Apply a spring force to a group of atoms or between two groups of atoms. This is useful for applying an umbrella force to a small molecule or lightly tethering a large group of atoms (e.g. all the solvent or a large molecule) to the center of the simulation box so that it doesn't wander away over the course of a long simulation. It can also be used to hold the centers of mass of two groups of atoms at a given distance or orientation with respect to each other.

The *tether* style attaches a spring between a fixed point *x,y,z* and the center of mass of the fix group of atoms. The equilibrium position of the spring is R0. At each timestep the distance R from the center of mass of the group of atoms to the tethering point is computed, taking account of wrap-around in a periodic simulation box. A restoring force of magnitude K (R - R0) Mi / M is applied to each atom in the group where *K* is the spring constant, Mi is the mass of the atom, and M is the total mass of all atoms in the group. Note that *K* thus represents the spring constant for the total force on the group of atoms, not for a spring applied to each atom.

The *couple* style links two groups of atoms together. The first group is the fix group; the second is specified by group-ID2. The groups are coupled together by a spring that is at equilibrium when the two groups are displaced by a vector *x,y,z* with respect to each other and at a distance R0 from that displacement. Note that *x,y,z* is the equilibrium displacement of group-ID2 relative to the fix group. Thus (1,1,0) is a different spring than (-1,-1,0). When the relative positions and distance between the two groups are not in equilibrium, the same spring force described above is applied to atoms in each of the two groups.

For both the *tether* and *couple* styles, any of the x,y,z values can be specified as NULL which means do not include that dimension in the distance calculation or force application.

The first example above pulls the ligand towards the point (0,0,0). The second example holds the ligand near the surface of a sphere of radius 5 around the point (0,0,0). The third example holds the ligand a distance 3 away from the z=2 plane (on either side).

The fourth example holds 2 bilayers a distance 10 apart in z. For the last two examples, imagine a pore (a slab of atoms with a cylindrical hole cut out) oriented with the pore axis along z, and an ion moving within the pore. The fifth example holds the ion a distance of -20 below the z = 0 center plane of the pore (umbrella sampling). The last example holds the ion a distance 5 away from the pore axis (assuming the center-of-mass of the pore in x,y is the pore axis).

Note: The center of mass of a group of atoms is calculated in "unwrapped" coordinates using atom image flags, which means that the group can straddle a periodic boundary. See the *dump* doc page for a discussion of unwrapped

coordinates. It also means that a spring connecting two groups or a group and the tether point can cross a periodic boundary and its length be calculated correctly.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify* *energy* option is supported by this fix to add the energy stored in the spring to the system's potential energy as part of *thermodynamic output*.

The *fix_modify* *respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix is adding its forces. Default is the outermost level.

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the spring energy = 0.5 * K * r^2.

This fix also computes global 4-vector which can be accessed by various *output commands*. The first 3 quantities in the vector are xyz components of the total force added to the group of atoms by the spring. In the case of the *couple* style, it is the force on the fix group (group-ID) or the negative of the force on the 2nd group (group-ID2). The 4th quantity in the vector is the magnitude of the force added by the spring, as a positive value if (r-R0) > 0 and a negative value if (r-R0) < 0. This sign convention can be useful when using the spring force to compute a potential of mean force (PMF).

The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command.

Note: If you want the spring energy to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the *fix_modify* *energy* option for this fix.

16.227.4 Restrictions

none

16.227.5 Related commands

fix drag, *fix spring/self*, *fix spring/rg*, *fix smd*

Default: none

16.228 fix spring/chunk command

16.228.1 Syntax

```
fix ID group-ID spring/chunk K chunkID comID
```

- ID, group-ID are documented in *fix* command
- spring/chunk = style name of this fix command
- K = spring constant for each chunk (force/distance units)

- chunkID = ID of *compute chunk/atom* command
- comID = ID of *compute com/chunk* command

16.228.2 Examples

```
fix restrain all spring/chunk 100 chunkID comID
```

16.228.3 Description

Apply a spring force to the center-of-mass (COM) of chunks of atoms as defined by the *compute chunk/atom* command. Chunks can be molecules or spatial bins or other groupings of atoms. This is a way of tethering each chunk to its initial COM coordinates.

The *chunkID* is the ID of a compute chunk/atom command defined in the input script. It is used to define the chunks. The *comID* is the ID of a compute com/chunk command defined in the input script. It is used to compute the COMs of each chunk.

At the beginning of the first *run* or *minimize* command after this fix is defined, the initial COM of each chunk is calculated and stored as R0m, where M is the chunk number. Thereafter, at every timestep (or minimization iteration), the current COM of each chunk is calculated as Rm. A restoring force of magnitude K (Rm - R0m) Mi / Mm is applied to each atom in each chunk where K is the specified spring constant, Mi is the mass of the atom, and Mm is the total mass of all atoms in the chunk. Note that K thus represents the spring constant for the total force on each chunk of atoms, not for a spring applied to each atom.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify* *energy* option is supported by this fix to add the energy stored in all the springs to the system's potential energy as part of *thermodynamic output*.

The *fix_modify* *respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix is adding its forces. Default is the outermost level.

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the energy of all the springs, i.e. 0.5 * K * r^2 per-spring.

The scalar value calculated by this fix is "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command.

Note: If you want the spring energies to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the *fix_modify* *energy* option for this fix.

16.228.4 Restrictions

none

16.228.5 Related commands

fix spring, *fix spring/self*, *fix spring/rg*

Default: none

16.229 fix spring/rg command

16.229.1 Syntax

```
fix ID group-ID spring/rg K RG0
```

- ID, group-ID are documented in *fix* command
- spring/rg = style name of this fix command
- K = harmonic force constant (force/distance units)
- RG0 = target radius of gyration to constrain to (distance units)

```
if RG0 = NULL, use the current RG as the target value
```

16.229.2 Examples

```
fix 1 protein spring/rg 5.0 10.0
fix 2 micelle spring/rg 5.0 NULL
```

16.229.3 Description

Apply a harmonic restraining force to atoms in the group to affect their central moment about the center of mass (radius of gyration). This fix is useful to encourage a protein or polymer to fold/unfold and also when sampling along the radius of gyration as a reaction coordinate (i.e. for protein folding).

The radius of gyration is defined as RG in the first formula. The energy of the constraint and associated force on each atom is given by the second and third formulas, when the group is at a different RG than the target value RG0.

$$
\begin{aligned}
{R_G}^2 &= \frac{1}{M}\sum_i^N m_i \left(x_i - \frac{1}{M}\sum_j^N m_j x_j\right)^2 \\
E &= K\left(R_G - R_{G0}\right)^2 \\
F_i &= 2K\frac{m_i}{M}\left(1 - \frac{R_{G0}}{R_G}\right)\left(x_i - \frac{1}{M}\sum_j^N m_j x_j\right)
\end{aligned}
$$

The (x_i - center-of-mass) term is computed taking into account periodic boundary conditions, m_i is the mass of the atom, and *M* is the mass of the entire group. Note that K is thus a force constant for the aggregate force on the group of atoms, not a per-atom force.

If R_{G0} is specified as NULL, then the RG of the group is computed at the time the fix is specified, and that value is used as the target.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

The *fix_modify* *respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix is adding its forces. Default is the outermost level.

16.229.4 Restrictions

none

16.229.5 Related commands

fix spring, *fix spring/self* *fix drag*, *fix smd*

Default: none

16.230 fix spring/self command

16.230.1 Syntax

```
fix ID group-ID spring/self K dir
```

- ID, group-ID are documented in *fix* command
- spring/self = style name of this fix command
- K = spring constant (force/distance units)
- dir = xyz, xy, xz, yz, x, y, or z (optional, default: xyz)

16.230.2 Examples

```
fix tether boundary-atoms spring/self 10.0
fix zrest  move spring/self 10.0 z
```

16.230.3 Description

Apply a spring force independently to each atom in the group to tether it to its initial position. The initial position for each atom is its location at the time the fix command was issued. At each timestep, the magnitude of the force on each atom is -Kr, where r is the displacement of the atom from its current position to its initial position. The distance r correctly takes into account any crossings of periodic boundary by the atom since it was in its initial position.

With the (optional) dir flag, one can select in which direction the spring force is applied. By default, the restraint is applied in all directions, but it can be limited to the xy-, xz-, yz-plane and the x-, y-, or z-direction, thus restraining the atoms to a line or a plane, respectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the original coordinates of tethered atoms to *binary restart files*, so that the spring effect will be the same in a restarted simulation. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix_modify* *energy* option is supported by this fix to add the energy stored in the per-atom springs to the system's potential energy as part of *thermodynamic output*.

The *fix_modify* *respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix is adding its forces. Default is the outermost level.

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is an energy which is the sum of the spring energy for each atom, where the per-atom energy is 0.5 * K * r^2. The scalar value calculated by this fix is "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command.

Note: If you want the per-atom spring energy to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the *fix_modify* *energy* option for this fix.

16.230.4 Restrictions

none

16.230.5 Related commands

fix drag, *fix spring*, *fix smd*, *fix spring/rg*

Default: none

16.231 fix srd command

16.231.1 Syntax

```
fix ID group-ID srd N groupbig-ID Tsrd hgrid seed keyword value ...
```

- ID, group-ID are documented in *fix* command
- srd = style name of this fix command
- N = reset SRD particle velocities every this many timesteps
- groupbig-ID = ID of group of large particles that SRDs interact with
- Tsrd = temperature of SRD particles (temperature units)
- hgrid = grid spacing for SRD grouping (distance units)
- seed = random # seed (positive integer)
- zero or more keyword/value pairs may be appended

- keyword = *lamda* or *collision* or *overlap* or *inside* or *exact* or *radius* or *bounce* or *search* or *cubic* or *shift* or *tstat* or *rescale*

```
lamda value = mean free path of SRD particles (distance units)
collision value = noslip or slip = collision model
overlap value = yes or no = whether big particles may overlap
inside value = error or warn or ignore = how SRD particles which end up␣
↪inside a big particle are treated
exact value = yes or no
radius value = rfactor = scale collision radius by this factor
bounce value = Nbounce = max # of collisions an SRD particle can undergo␣
↪in one timestep
search value = sgrid = grid spacing for collision partner searching␣
↪(distance units)
cubic values = style tolerance
  style = error or warn
  tolerance = fractional difference allowed (0 <= tol <= 1)
shift values = flag shiftseed
  flag = yes or no or possible = SRD bin shifting for better statistics
    yes = perform bin shifting each time SRD velocities are rescaled
    no = no shifting
    possible = shift depending on mean free path and bin size
  shiftseed = random # seed (positive integer)
tstat value = yes or no = thermostat SRD particles or not
rescale value = yes or no or rotate or collide = rescaling of SRD␣
↪velocities
  yes = rescale during velocity rotation and collisions
  no = no rescaling
  rotate = rescale during velocity rotation, but not collisions
  collide = rescale during collisions, but not velocity rotation
```

16.231.2 Examples

```
fix 1 srd srd 10 big 1.0 0.25 482984
fix 1 srd srd 10 big 0.5 0.25 482984 collision slip search 0.5
```

16.231.3 Description

Treat a group of particles as stochastic rotation dynamics (SRD) particles that serve as a background solvent when interacting with big (colloidal) particles in groupbig-ID. The SRD formalism is described in *(Hecht)*. The key idea behind using SRD particles as a cheap coarse-grained solvent is that SRD particles do not interact with each other, but only with the solute particles, which in LAMMPS can be spheroids, ellipsoids, or line segments, or triangles, or rigid bodies containing multiple spheroids or ellipsoids or line segments or triangles. The collision and rotation properties of the model imbue the SRD particles with fluid-like properties, including an effective viscosity. Thus simulations with large solute particles can be run more quickly, to measure solute properties like diffusivity and viscosity in a background fluid. The usual LAMMPS fixes for such simulations, such as *fix deform*, *fix viscosity*, and *fix nvt/sllod*, can be used in conjunction with the SRD model.

For more details on how the SRD model is implemented in LAMMPS, *this paper* describes the implementation and usage of pure SRD fluids. *This paper*, which is nearly complete, describes the implementation and usage of mixture systems (solute particles in an SRD fluid). See the examples/srd directory for sample input scripts using SRD particles in both settings.

This fix does two things:

1. It advects the SRD particles, performing collisions between SRD and big particles or walls every timestep, imparting force and torque to the big particles. Collisions also change the position and velocity of SRD particles.
2. It resets the velocity distribution of SRD particles via random rotations every N timesteps.

SRD particles have a mass, temperature, characteristic timestep dt_{SRD}, and mean free path between collisions (λ). The fundamental equation relating these 4 quantities is

$$\lambda = dt_{SRD}\sqrt{\frac{k_B T_{SRD}}{m}}$$

The mass *m* of SRD particles is set by the *mass* command elsewhere in the input script. The SRD timestep dt_{SRD} is N times the step *dt* defined by the *timestep* command. Big particles move in the normal way via a time integration *fix* with a short timestep dt. SRD particles advect with a large timestep $dt_{SRD} \geq dt$.

If the *lamda* keyword is not specified, the SRD temperature T_{SRD} is used in the above formula to compute λ. If the *lamda* keyword is specified, then the *Tsrd* setting is ignored and the above equation is used to compute the SRD temperature.

The characteristic length scale for the SRD fluid is set by *hgrid* which is used to bin SRD particles for purposes of resetting their velocities. Normally hgrid is set to be 1/4 of the big particle diameter or smaller, to adequately resolve fluid properties around the big particles.

λ cannot be smaller than 0.6 * hgrid, else an error is generated (unless the *shift* keyword is used, see below). The velocities of SRD particles are bounded by Vmax, which is set so that an SRD particle will not advect further than $D_{max} = 4\lambda$ in dt_{SRD}. This means that roughly speaking, D_{max} should not be larger than a big particle diameter, else SRDs may pass through big particles without colliding. A warning is generated if this is the case.

Collisions between SRD particles and big particles or walls are modeled as a lightweight SRD point particle hitting a heavy big particle of given diameter or a wall at a point on its surface and bouncing off with a new velocity. The collision changes the momentum of the SRD particle. It imparts a force and torque to the big particle. It imparts a force to a wall. Static or moving SRD walls are setup via the *fix wall/srd* command. For the remainder of this doc page, a collision of an SRD particle with a wall can be viewed as a collision with a big particle of infinite radius and mass.

The *collision* keyword sets the style of collisions. The *slip* style means that the tangential component of the SRD particle momentum is preserved. Thus a force is imparted to a big particle, but no torque. The normal component of the new SRD velocity is sampled from a Gaussian distribution at temperature *Tsrd*.

For the *noslip* style, both the normal and tangential components of the new SRD velocity are sampled from a Gaussian distribution at temperature *Tsrd*. Additionally, a new tangential direction for the SRD velocity is chosen randomly. This collision style imparts torque to a big particle. Thus a time integrator *fix* that rotates the big particles appropriately should be used.

The *overlap* keyword should be set to *yes* if two (or more) big particles can ever overlap. This depends on the pair potential interaction used for big-big interactions, or could be the case if multiple big particles are held together as rigid bodies via the *fix rigid* command. If the *overlap* keyword is *no* and big particles do in fact overlap, then SRD/big collisions can generate an error if an SRD ends up inside two (or more) big particles at once. How this error is treated is determined by the *inside* keyword. Running with *overlap* set to *no* allows for faster collision checking, so it should only be set to *yes* if needed.

The *inside* keyword determines how a collision is treated if the computation determines that the timestep started with the SRD particle already inside a big particle. If the setting is *error* then this generates an error message and LAMMPS stops. If the setting is *warn* then this generates a warning message and the code continues. If the setting is *ignore* then no message is generated. One of the output quantities logged by the fix (see below) tallies the number of such events, so it can be monitored. Note that once an SRD particle is inside a big particle, it may remain there for several steps until it drifts outside the big particle.

The *exact* keyword determines how accurately collisions are computed. A setting of *yes* computes the time and position of each collision as SRD and big particles move together. A setting of *no* estimates the position of each collision based on the end-of-timestep positions of the SRD and big particle. If *overlap* is set to yes, the setting of the *exact* keyword is ignored since time-accurate collisions are needed.

The *radius* keyword scales the effective size of big particles. If big particles will overlap as they undergo dynamics, then this keyword can be used to scale down their effective collision radius by an amount *rfactor*, so that SRD particle will only collide with one big particle at a time. For example, in a Lennard-Jones system at a temperature of 1.0 (in reduced LJ units), the minimum separation between two big particles is as small as about 0.88 sigma. Thus an *rfactor* value of 0.85 should prevent dual collisions.

The *bounce* keyword can be used to limit the maximum number of collisions an SRD particle undergoes in a single timestep as it bounces between nearby big particles. Note that if the limit is reached, the SRD can be left inside a big particle. A setting of 0 is the same as no limit.

There are 2 kinds of bins created and maintained when running an SRD simulation. The first are "SRD bins" which are used to bin SRD particles and reset their velocities, as discussed above. The second are "search bins" which are used to identify SRD/big particle collisions.

The *search* keyword can be used to choose a search bin size for identifying SRD/big particle collisions. The default is to use the *hgrid* parameter for SRD bins as the search bin size. Choosing a smaller or large value may be more efficient, depending on the problem. But, in a statistical sense, it should not change the simulation results.

The *cubic* keyword can be used to generate an error or warning when the bin size chosen by LAMMPS creates SRD bins that are non-cubic or different than the requested value of *hgrid* by a specified *tolerance*. Note that using non-cubic SRD bins can lead to undetermined behavior when rotating the velocities of SRD particles, hence LAMMPS tries to protect you from this problem.

LAMMPS attempts to set the SRD bin size to exactly *hgrid*. However, there must be an integer number of bins in each dimension of the simulation box. Thus the actual bin size will depend on the size and shape of the overall simulation box. The actual bin size is printed as part of the SRD output when a simulation begins.

If the actual bin size in non-cubic by an amount exceeding the tolerance, an error or warning is printed, depending on the style of the *cubic* keyword. Likewise, if the actual bin size differs from the requested *hgrid* value by an amount exceeding the tolerance, then an error or warning is printed. The *tolerance* is a fractional difference. E.g. a tolerance setting of 0.01 on the shape means that if the ratio of any 2 bin dimensions exceeds (1 +/- tolerance) then an error or warning is generated. Similarly, if the ratio of any bin dimension with *hgrid* exceeds (1 +/- tolerance), then an error or warning is generated.

Note: The fix srd command can be used with simulations the size and/or shape of the simulation box changes. This can be due to non-periodic boundary conditions or the use of fixes such as the *fix deform* or *fix wall/srd* commands to impose a shear on an SRD fluid or an interaction with an external wall. If the box size changes then the size of SRD bins must be recalculated every reneighboring. This is not necessary if only the box shape changes. This re-binning is always done so as to fit an integer number of bins in the current box dimension, whether it be a fixed, shrink-wrapped, or periodic boundary, as set by the *boundary* command. If the box size or shape changes, then the size of the search bins must be recalculated every reneighboring. Note that changing the SRD bin size may alter the properties of the SRD fluid, such as its viscosity.

The *shift* keyword determines whether the coordinates of SRD particles are randomly shifted when binned for purposes of rotating their velocities. When no shifting is performed, SRD particles are binned and the velocity distribution of the set of SRD particles in each bin is adjusted via a rotation operator. This is a statistically valid operation if SRD particles move sufficiently far between successive rotations. This is determined by their mean-free path λ. If λ is less than 0.6 of the SRD bin size, then shifting is required. A shift means that all of the SRD particles are shifted by a vector whose coordinates are chosen randomly in the range [-1/2 bin size, 1/2 bin size]. Note that all particles are

shifted by the same vector. The specified random number *shiftseed* is used to generate these vectors. This operation sufficiently randomizes which SRD particles are in the same bin, even if $lambda$ is small.

If the *shift* flag is set to *no*, then no shifting is performed, but bin data will be communicated if bins overlap processor boundaries. An error will be generated if $\lambda < 0.6$ of the SRD bin size. If the *shift* flag is set to *possible*, then shifting is performed only if $\lambda < 0.6$ of the SRD bin size. A warning is generated to let you know this is occurring. If the *shift* flag is set to *yes* then shifting is performed regardless of the magnitude of λ. Note that the *shiftseed* is not used if the *shift* flag is set to *no*, but must still be specified.

Note that shifting of SRD coordinates requires extra communication, hence it should not normally be enabled unless required.

The *tstat* keyword will thermostat the SRD particles to the specified *Tsrd*. This is done every N timesteps, during the velocity rotation operation, by rescaling the thermal velocity of particles in each SRD bin to the desired temperature. If there is a streaming velocity associated with the system, e.g. due to use of the *fix deform* command to perform a simulation undergoing shear, then that is also accounted for. The mean velocity of each bin of SRD particles is set to the position-dependent streaming velocity, based on the coordinates of the center of the SRD bin. Note that collisions of SRD particles with big particles or walls has a thermostatting effect on the colliding particles, so it may not be necessary to thermostat the SRD particles on a bin by bin basis in that case. Also note that for streaming simulations, if no thermostatting is performed (the default), then it may take a long time for the SRD fluid to come to equilibrium with a velocity profile that matches the simulation box deformation.

The *rescale* keyword enables rescaling of an SRD particle's velocity if it would travel more than 4 mean-free paths in an SRD timestep. If an SRD particle exceeds this velocity it is possible it will be lost when migrating to other processors or that collisions with big particles will be missed, either of which will generate errors. Thus the safest mode is to run with rescaling enabled. However rescaling removes kinetic energy from the system (the particle's velocity is reduced). The latter will not typically be a problem if thermostatting is enabled via the *tstat* keyword or if SRD collisions with big particles or walls effectively thermostat the system. If you wish to turn off rescaling (on is the default), e.g. for a pure SRD system with no thermostatting so that the temperature does not decline over time, the *rescale* keyword can be used. The *no* value turns rescaling off during collisions and the per-bin velocity rotation operation. The *collide* and *rotate* values turn it on for one of the operations and off for the other.

Note: This fix is normally used for simulations with a huge number of SRD particles relative to the number of big particles, e.g. 100 to 1. In this scenario, computations that involve only big particles (neighbor list creation, communication, time integration) can slow down dramatically due to the large number of background SRD particles.

Three other input script commands will largely overcome this effect, speeding up an SRD simulation by a significant amount. These are the *atom_modify first*, *neigh_modify include*, and *comm_modify group* commands. Each takes a group-ID as an argument, which in this case should be the group-ID of the big solute particles.

Additionally, when a *pair_style* for big/big particle interactions is specified, the *pair_coeff* command should be used to turn off big/SRD interactions, e.g. by setting their epsilon or cutoff length to 0.0.

The "delete_atoms overlap" command may be useful in setting up an SRD simulation to insure there are no initial overlaps between big and SRD particles.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix tabulates several SRD statistics which are stored in a vector of length 12, which can be accessed by various *output commands*. The vector values calculated by this fix are "intensive", meaning they do not scale with the size of the simulation. Technically, the first 8 do scale with the size of the simulation, but treating them as intensive means they are not scaled when printed as part of thermodynamic output.

These are the 12 quantities. All are values for the current timestep, except for quantity 5 and the last three, each of which are cumulative quantities since the beginning of the run.

- (1) # of SRD/big collision checks performed
- (2) # of SRDs which had a collision
- (3) # of SRD/big collisions (including multiple bounces)
- (4) # of SRD particles inside a big particle
- (5) # of SRD particles whose velocity was rescaled to be < Vmax
- (6) # of bins for collision searching
- (7) # of bins for SRD velocity rotation
- (8) # of bins in which SRD temperature was computed
- (9) SRD temperature
- (10) # of SRD particles which have undergone max # of bounces
- (11) max # of bounces any SRD particle has had in a single step
- (12) # of reneighborings due to SRD particles moving too far

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.231.4 Restrictions

This command can only be used if LAMMPS was built with the SRD package. See the *Build package* doc page for more info.

16.231.5 Related commands

fix wall/srd

16.231.6 Default

The option defaults are: *lamda* (λ) is inferred from *Tsrd*, collision = noslip, overlap = no, inside = error, exact = yes, radius = 1.0, bounce = 0, search = hgrid, cubic = error 0.01, shift = no, tstat = no, and rescale = yes.

(Hecht) Hecht, Harting, Ihle, Herrmann, Phys Rev E, 72, 011408 (2005).

(Petersen) Petersen, Lechman, Plimpton, Grest, in' t Veld, Schunk, J Chem Phys, 132, 174106 (2010).

(Lechman) Lechman, et al, in preparation (2010).

16.232 fix store/force command

16.232.1 Syntax

```
fix ID group-ID store/force
```

- ID, group-ID are documented in *fix* command
- store/force = style name of this fix command

16.232.2 Examples

```
fix 1 all store/force
```

16.232.3 Description

Store the forces on atoms in the group at the point during each timestep when the fix is invoked, as described below. This is useful for storing forces before constraints or other boundary conditions are computed which modify the forces, so that unmodified forces can be *written to a dump file* or accessed by other *output commands* that use per-atom quantities.

This fix is invoked at the point in the velocity-Verlet timestepping immediately after *pair*, *bond*, *angle*, *dihedral*, *improper*, and *long-range* forces have been calculated. It is the point in the timestep when various fixes that compute constraint forces are calculated and potentially modify the force on each atom. Examples of such fixes are *fix shake*, *fix wall*, and *fix indent*.

Note: The order in which various fixes are applied which operate at the same point during the timestep, is the same as the order they are specified in the input script. Thus normally, if you want to store per-atom forces due to force field interactions, before constraints are applied, you should list this fix first within that set of fixes, i.e. before other fixes that apply constraints. However, if you wish to include certain constraints (e.g. fix shake) in the stored force, then it could be specified after some fixes and before others.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix produces a per-atom array which can be accessed by various *output commands*. The number of columns for each atom is 3, and the columns store the x,y,z forces on each atom. The per-atom values be accessed on any timestep.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.232.4 Restrictions

none

16.232.5 Related commands

fix store_state

Default: none

16.233 fix store/state command

16.233.1 Syntax

```
fix ID group-ID store/state N input1 input2 ... keyword value ...
```

- ID, group-ID are documented in *fix* command
- store/state = style name of this fix command
- N = store atom attributes every N steps, N = 0 for initial store only
- input = one or more atom attributes

```
possible attributes = id, mol, type, mass,
                      x, y, z, xs, ys, zs, xu, yu, zu, xsu, ysu, zsu, ix, iy, iz,
                      vx, vy, vz, fx, fy, fz,
                      q, mux, muy, muz, mu,
                      radius, diameter, omegax, omegay, omegaz,
                      angmomx, angmomy, angmomz, tqx, tqy, tqz,
                      c_ID, c_ID[N], f_ID, f_ID[N], v_name,
                      d_name, i_name
```

```
id = atom ID
mol = molecule ID
type = atom type
mass = atom mass
x,y,z = unscaled atom coordinates
xs,ys,zs = scaled atom coordinates
xu,yu,zu = unwrapped atom coordinates
xsu,ysu,zsu = scaled unwrapped atom coordinates
ix,iy,iz = box image that the atom is in
vx,vy,vz = atom velocities
fx,fy,fz = forces on atoms
q = atom charge
mux,muy,muz = orientation of dipolar atom
mu = magnitued of dipole moment of atom
radius,diameter = radius.diameter of spherical particle
omegax,omegay,omegaz = angular velocity of spherical particle
angmomx,angmomy,angmomz = angular momentum of aspherical particle
tqx,tqy,tqz = torque on finite-size particles
c_ID = per-atom vector calculated by a compute with ID
c_ID[I] = Ith column of per-atom array calculated by a compute with ID
f_ID = per-atom vector calculated by a fix with ID
```

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```
f_ID[I] = Ith column of per-atom array calculated by a fix with ID
v_name = per-atom vector calculated by an atom-style variable with name
d_name = per-atom floating point vector name, managed by fix property/atom
i_name = per-atom integer vector name, managed by fix property/atom
```

- zero or more keyword/value pairs may be appended
- keyword = *com*

  com value = *yes* or *no*

16.233.2 Examples

```
fix 1 all store/state 0 x y z
fix 1 all store/state 0 xu yu zu com yes
fix 2 all store/state 1000 vx vy vz
```

16.233.3 Description

Define a fix that stores attributes for each atom in the group at the time the fix is defined. If *N* is 0, then the values are never updated, so this is a way of archiving an atom attribute at a given time for future use in a calculation or output. See the discussion of *output commands* that take fixes as inputs.

If *N* is not zero, then the attributes will be updated every *N* steps.

Note: Actually, only atom attributes specified by keywords like *xu* or *vy* or *radius* are initially stored immediately at the point in your input script when the fix is defined. Attributes specified by a compute, fix, or variable are not initially stored until the first run following the fix definition begins. This is because calculating those attributes may require quantities that are not defined in between runs.

The list of possible attributes is the same as that used by the *dump custom* command, which describes their meaning.

If the *com* keyword is set to *yes* then the *xu*, *yu*, and *zu* inputs store the position of each atom relative to the center-of-mass of the group of atoms, instead of storing the absolute position.

The requested values are stored in a per-atom vector or array as discussed below. Zeroes are stored for atoms not in the specified group.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the per-atom values it stores to *binary restart files*, so that the values can be restored when a simulation is restarted. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

None of the *fix_modify* options are relevant to this fix.

If a single input is specified, this fix produces a per-atom vector. If multiple inputs are specified, a per-atom array is produced where the number of columns for each atom is the number of inputs. These can be accessed by various *output commands*. The per-atom values be accessed on any timestep.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.233.4 Restrictions

none

16.233.5 Related commands

dump custom, *compute property/atom*, *fix property/atom*, *variable*

16.233.6 Default

The option default is com = no.

16.234 fix temp/berendsen command

16.234.1 Syntax

```
fix ID group-ID temp/berendsen Tstart Tstop Tdamp
```

- ID, group-ID are documented in *fix* command
- temp/berendsen = style name of this fix command
- Tstart,Tstop = desired temperature at start/end of run

  ```
  Tstart can be a variable (see below)
  ```

- Tdamp = temperature damping parameter (time units)

16.234.2 Examples

```
fix 1 all temp/berendsen 300.0 300.0 100.0
```

16.234.3 Description

Reset the temperature of a group of atoms by using a Berendsen thermostat *(Berendsen)*, which rescales their velocities every timestep.

The thermostat is applied to only the translational degrees of freedom for the particles, which is an important consideration for finite-size particles which have rotational degrees of freedom are being thermostatted with this fix. The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

The desired temperature at each timestep is a ramped value during the run from *Tstart* to *Tstop*. The *Tdamp* parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 100.0 means to relax the temperature in a timespan of (roughly) 100 time units (tau or fmsec or psec - see the *units* command).

Tstart can be specified as an equal-style *variable*. In this case, the *Tstop* setting is ignored. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the target temperature.

Note: This thermostat will generate an error if the current temperature is zero at the end of a timestep. It cannot rescale a zero temperature.

Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent temperature.

Note: Unlike the *fix nvt* command which performs Nose/Hoover thermostatting AND time integration, this fix does NOT perform time integration. It only modifies velocities to effect thermostatting. Thus you must use a separate time integration fix, like *fix nve* to actually update the positions of atoms using the modified velocities. Likewise, this fix should not normally be used on atoms that also have their temperature controlled by another fix - e.g. by *fix nvt* or *fix langevin* commands.

See the *Howto thermostat* doc page for a discussion of different ways to compute temperature and perform thermostatting.

This fix computes a temperature each timestep. To do this, the fix creates its own compute of style "temp", as if this command had been issued:

```
compute fix-ID_temp group-ID temp
```

See the *compute temp* command for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp*. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the *compute_modify* command or print this temperature during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with *compute commands* that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the *fix_modify* command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual *compute commands* to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify temp* option is supported by this fix. You can use it to assign a temperature *compute* you have defined to this fix which will be used in its thermostatting procedure, as described above. For consistency, the group used by this fix and by the compute should be the same.

The *fix_modify energy* option is supported by this fix to add the energy change implied by a velocity rescaling to the system's potential energy as part of *thermodynamic output*.

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the cumulative energy change due to this fix. The scalar value calculated by this fix is "extensive".

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.234.4 Restrictions

This fix can be used with dynamic groups as defined by the *group* command. Likewise it can be used with groups to which atoms are added or deleted over time, e.g. a deposition simulation. However, the conservation properties of the thermostat and barostat are defined for systems with a static set of atoms. You may observe odd behavior if the atoms in a group vary dramatically over time or the atom count becomes very small.

16.234.5 Related commands

fix nve, *fix nvt*, *fix temp/rescale*, *fix langevin*, *fix_modify*, *compute temp*, *fix press/berendsen*

Default: none

(Berendsen) Berendsen, Postma, van Gunsteren, DiNola, Haak, J Chem Phys, 81, 3684 (1984).

16.235 fix temp/csvr command

16.236 fix temp/csld command

16.236.1 Syntax

```
fix ID group-ID temp/csvr Tstart Tstop Tdamp seed

fix ID group-ID temp/csld Tstart Tstop Tdamp seed
```

- ID, group-ID are documented in *fix* command
- temp/csvr or temp/csld = style name of this fix command
- Tstart,Tstop = desired temperature at start/end of run

  ```
  Tstart can be a variable (see below)
  ```

- Tdamp = temperature damping parameter (time units)
- seed = random number seed to use for white noise (positive integer)

16.236.2 Examples

```
fix 1 all temp/csvr 300.0 300.0 100.0 54324

fix 1 all temp/csld 100.0 300.0 10.0 123321
```

16.236.3 Description

Adjust the temperature with a canonical sampling thermostat that uses global velocity rescaling with Hamiltonian dynamics (*temp/csvr*) *(Bussi1)*, or Langevin dynamics (*temp/csld*) *(Bussi2)*. In the case of *temp/csvr* the thermostat is similar to the empirical Berendsen thermostat in *temp/berendsen*, but chooses the actual scaling factor from a suitably chosen (gaussian) distribution rather than having it determined from the time constant directly. In the case of *temp/csld* the velocities are updated to a linear combination of the current velocities with a gaussian distribution of velocities at the desired temperature. Both thermostats are applied every timestep.

The thermostat is applied to only the translational degrees of freedom for the particles, which is an important consideration for finite-size particles which have rotational degrees of freedom are being thermostatted with these fixes. The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

The desired temperature at each timestep is a ramped value during the run from *Tstart* to *Tstop*. The *Tdamp* parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 100.0 means to relax the temperature in a timespan of (roughly) 100 time units (tau or fmsec or psec - see the *units* command).

Tstart can be specified as an equal-style *variable*. In this case, the *Tstop* setting is ignored. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the target temperature.

Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent temperature.

Note: Unlike the *fix nvt* command which performs Nose/Hoover thermostatting AND time integration, these fixes do NOT perform time integration. They only modify velocities to effect thermostatting. Thus you must use a separate time integration fix, like *fix nve* to actually update the positions of atoms using the modified velocities. Likewise, these fixes should not normally be used on atoms that also have their temperature controlled by another fix - e.g. by *fix nvt* or *fix langevin* commands.

See the *Howto thermostat* doc page for a discussion of different ways to compute temperature and perform thermostatting.

These fixes compute a temperature each timestep. To do this, the fix creates its own compute of style "temp", as if this command had been issued:

```
compute fix-ID_temp group-ID temp
```

See the *compute temp* command for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp*. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the *compute_modify* command or print this temperature during thermodynamic output via the *thermo_style custom* command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* will have no effect on this fix.

Like other fixes that perform thermostatting, these fixes can be used with *compute commands* that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the *fix_modify* command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual *compute commands* to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Restart, fix_modify, output, run start/stop, minimize info:

No information about these fixes are written to *binary restart files*.

The *fix_modify* *temp* option is supported by these fixes. You can use it to assign a temperature *compute* you have defined to these fixes which will be used in its thermostatting procedure, as described above. For consistency, the group used by these fixes and by the compute should be the same.

These fixes can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

These fixes are not invoked during *energy minimization*.

These fixes compute a global scalar which can be accessed by various *output commands*. The scalar is the cumulative energy change due to the fix. The scalar value calculated by this fix is "extensive".

16.236.4 Restrictions

These fixes are not compatible with *fix shake*.

The fix can be used with dynamic groups as defined by the *group* command. Likewise it can be used with groups to which atoms are added or deleted over time, e.g. a deposition simulation. However, the conservation properties of the thermostat and barostat are defined for systems with a static set of atoms. You may observe odd behavior if the atoms in a group vary dramatically over time or the atom count becomes very small.

16.236.5 Related commands

fix nve, *fix nvt*, *fix temp/rescale*, *fix langevin*, *fix_modify*, *compute temp*, *fix temp/berendsen*

Default: none

(Bussi1) Bussi, Donadio and Parrinello, J. Chem. Phys. 126, 014101(2007)

(Bussi2) Bussi and Parrinello, Phys. Rev. E 75, 056707 (2007)

16.237 fix temp/rescale command

16.237.1 Syntax

```
fix ID group-ID temp/rescale N Tstart Tstop window fraction
```

- ID, group-ID are documented in *fix* command
- temp/rescale = style name of this fix command
- N = perform rescaling every N steps
- Tstart,Tstop = desired temperature at start/end of run (temperature units)

  ```
  Tstart can be a variable (see below)
  ```

- window = only rescale if temperature is outside this window (temperature units)
- fraction = rescale to target temperature by this fraction

16.237.2 Examples

```
fix 3 flow temp/rescale 100 1.0 1.1 0.02 0.5
fix 3 boundary temp/rescale 1 1.0 1.5 0.05 1.0
fix 3 boundary temp/rescale 1 1.0 1.5 0.05 1.0
```

16.237.3 Description

Reset the temperature of a group of atoms by explicitly rescaling their velocities.

The rescaling is applied to only the translational degrees of freedom for the particles, which is an important consideration if finite-size particles which have rotational degrees of freedom are being thermostatted with this fix. The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

Rescaling is performed every N timesteps. The target temperature is a ramped value between the *Tstart* and *Tstop* temperatures at the beginning and end of the run.

Note: This thermostat will generate an error if the current temperature is zero at the end of a timestep it is invoked on. It cannot rescale a zero temperature.

Tstart can be specified as an equal-style *variable*. In this case, the *Tstop* setting is ignored. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the target temperature.

Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent temperature.

Rescaling is only performed if the difference between the current and desired temperatures is greater than the *window* value. The amount of rescaling that is applied is a *fraction* (from 0.0 to 1.0) of the difference between the actual and desired temperature. E.g. if *fraction* = 1.0, the temperature is reset to exactly the desired value.

Note: Unlike the *fix nvt* command which performs Nose/Hoover thermostatting AND time integration, this fix does NOT perform time integration. It only modifies velocities to effect thermostatting. Thus you must use a separate time integration fix, like *fix nve* to actually update the positions of atoms using the modified velocities. Likewise, this fix should not normally be used on atoms that also have their temperature controlled by another fix - e.g. by *fix nvt* or *fix langevin* commands.

See the *Howto thermostat* doc page for a discussion of different ways to compute temperature and perform thermostatting.

This fix computes a temperature each timestep. To do this, the fix creates its own compute of style "temp", as if one of this command had been issued:

```
compute fix-ID_temp group-ID temp
```

See the *compute temp* for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the *thermo_style* command) with ID = *thermo_temp*. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the *compute_modify* command or print this temperature during thermodynamic output via the *thermo_style custom*

command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with *compute commands* that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the *fix_modify* command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual *compute commands* to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify* *temp* option is supported by this fix. You can use it to assign a temperature *compute* you have defined to this fix which will be used in its thermostatting procedure, as described above. For consistency, the group used by this fix and by the compute should be the same.

The *fix_modify* *energy* option is supported by this fix to add the energy change implied by a velocity rescaling to the system's potential energy as part of *thermodynamic output*.

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the cumulative energy change due to this fix. The scalar value calculated by this fix is "extensive".

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.237.4 Restrictions

none

16.237.5 Related commands

fix langevin, *fix nvt*, *fix_modify*

Default: none

16.238 fix temp/rescale/eff command

16.238.1 Syntax

```
fix ID group-ID temp/rescale/eff N Tstart Tstop window fraction
```

- ID, group-ID are documented in *fix* command
- temp/rescale/eff = style name of this fix command
- N = perform rescaling every N steps
- Tstart,Tstop = desired temperature at start/end of run (temperature units)

- window = only rescale if temperature is outside this window (temperature units)
- fraction = rescale to target temperature by this fraction

16.238.2 Examples

```
fix 3 flow temp/rescale/eff 10 1.0 100.0 0.02 1.0
```

16.238.3 Description

Reset the temperature of a group of nuclei and electrons in the *electron force field* model by explicitly rescaling their velocities.

The operation of this fix is exactly like that described by the *fix temp/rescale* command, except that the rescaling is also applied to the radial electron velocity for electron particles.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify* *temp* option is supported by this fix. You can use it to assign a temperature *compute* you have defined to this fix which will be used in its thermostatting procedure, as described above. For consistency, the group used by this fix and by the compute should be the same.

The *fix_modify* *energy* option is supported by this fix to add the energy change implied by a velocity rescaling to the system's potential energy as part of *thermodynamic output*.

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the cumulative energy change due to this fix. The scalar value calculated by this fix is "extensive".

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.238.4 Restrictions

This fix is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.238.5 Related commands

fix langevin/eff, *fix nvt/eff*, *fix_modify*, *fix temp rescale*,

Default: none

16.239 fix tfmc command

16.239.1 Syntax

```
fix ID group-ID tfmc Delta Temp seed keyword value
```

- ID, group-ID are documented in *fix* command
- tfmc = style name of this fix command
- Delta = maximal displacement length (distance units)
- Temp = imposed temperature of the system
- seed = random number seed (positive integer)
- zero or more keyword/arg pairs may be appended
- keyword = *com* or *rot*

```
com args = xflag yflag zflag
  xflag,yflag,zflag = 0/1 to exclude/include each dimension
rot args = none
```

16.239.2 Examples

```
fix 1 all tfmc 0.1 1000.0 159345
fix 1 all tfmc 0.05 600.0 658943 com 1 1 0
fix 1 all tfmc 0.1 750.0 387068 com 1 1 1 rot
```

16.239.3 Description

Perform uniform-acceptance force-bias Monte Carlo (fbMC) simulations, using the time-stamped force-bias Monte Carlo (tfMC) algorithm described in *(Mees)* and *(Bal)*.

One successful use case of force-bias Monte Carlo methods is that they can be used to extend the time scale of atomistic simulations, in particular when long time scale relaxation effects must be considered; some interesting examples are given in the review by *(Neyts)*. An example of a typical use case would be the modelling of chemical vapor deposition (CVD) processes on a surface, in which impacts by gas-phase species can be performed using MD, but subsequent relaxation of the surface is too slow to be done using MD only. Using tfMC can allow for a much faster relaxation of the surface, so that higher fluxes can be used, effectively extending the time scale of the simulation. (Such an alternating simulation approach could be set up using a *loop*.)

The initial version of tfMC algorithm in *(Mees)* contained an estimation of the effective time scale of such a simulation, but it was later shown that the speed-up one can gain from a tfMC simulation is system- and process-dependent, ranging from none to several orders of magnitude. In general, solid-state processes such as (re)crystallization or growth can be accelerated by up to two or three orders of magnitude, whereas diffusion in the liquid phase is not accelerated at all. The observed pseudodynamics when using the tfMC method is not the actual dynamics one would obtain using MD, but the relative importance of processes can match the actual relative dynamics of the system quite well, provided *Delta* is chosen with care. Thus, the system's equilibrium is reached faster than in MD, along a path that is generally roughly similar to a typical MD simulation (but not necessarily so). See *(Bal)* for details.

Each step, all atoms in the selected group are displaced using the stochastic tfMC algorithm, which is designed to sample the canonical (NVT) ensemble at the temperature *Temp*. Although tfMC is a Monte Carlo algorithm and thus strictly speaking does not perform time integration, it is similar in the sense that it uses the forces on all atoms in order

to update their positions. Therefore, it is implemented as a time integration fix, and no other fixes of this type (such as *fix nve*) should be used at the same time. Because velocities do not play a role in this kind of Monte Carlo simulations, instantaneous temperatures as calculated by *temperature computes* or *thermodynamic output* have no meaning: the only relevant temperature is the sampling temperature *Temp*. Similarly, performing tfMC simulations does not require setting a *timestep* and the *simulated time* as calculated by LAMMPS is meaningless.

The critical parameter determining the success of a tfMC simulation is *Delta*, the maximal displacement length of the lightest element in the system: the larger it is, the longer the effective time scale of the simulation will be (there is an approximately quadratic dependence). However, *Delta* must also be chosen sufficiently small in order to comply with detailed balance; in general values between 5 and 10 % of the nearest neighbor distance are found to be a good choice. For a more extensive discussion with specific examples, please refer to *(Bal)*, which also describes how the code calculates element-specific maximal displacements from *Delta*, based on the fourth root of their mass.

Because of the uncorrelated movements of the atoms, the center-of-mass of the fix group will not necessarily be stationary, just like its orientation. When the *com* keyword is used, all atom positions will be shifted (after every tfMC iteration) in order to fix the position of the center-of-mass along the included directions, by setting the corresponding flag to 1. The *rot* keyword does the same for the rotational component of the tfMC displacements after every iteration.

Note: the *com* and *rot* keywords should not be used if an external force is acting on the specified fix group, along the included directions. This can be either a true external force (e.g. through *fix wall*) or forces due to the interaction with atoms not included in the fix group. This is because in such cases, translations or rotations of the fix group could be induced by these external forces, and removing them will lead to a violation of detailed balance.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

None of the *fix_modify* options are relevant to this fix.

This fix is not invoked during *energy minimization*.

16.239.4 Restrictions

This fix is part of the MC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix is not compatible with *fix shake*.

16.239.5 Related commands

fix gcmc, *fix nvt*

16.239.6 Default

The option default is com = 0 0 0

(Bal) K. M Bal and E. C. Neyts, J. Chem. Phys. 141, 204104 (2014).

(Mees) M. J. Mees, G. Pourtois, E. C. Neyts, B. J. Thijsse, and A. Stesmans, Phys. Rev. B 85, 134301 (2012).

(Neyts) E. C. Neyts and A. Bogaerts, Theor. Chem. Acc. 132, 1320 (2013).

16.240 fix thermal/conductivity command

16.240.1 Syntax

```
fix ID group-ID thermal/conductivity N edim Nbin keyword value ...
```

- ID, group-ID are documented in *fix* command
- thermal/conductivity = style name of this fix command
- N = perform kinetic energy exchange every N steps
- edim = *x* or *y* or *z* = direction of kinetic energy transfer
- Nbin = # of layers in edim direction (must be even number)
- zero or more keyword/value pairs may be appended
- keyword = *swap*

  swap value = Nswap = number of swaps to perform every N steps

16.240.2 Examples

```
fix 1 all thermal/conductivity 100 z 20
fix 1 all thermal/conductivity 50 z 20 swap 2
```

16.240.3 Description

Use the Muller-Plathe algorithm described in *this paper* to exchange kinetic energy between two particles in different regions of the simulation box every N steps. This induces a temperature gradient in the system. As described below this enables the thermal conductivity of a material to be calculated. This algorithm is sometimes called a reverse non-equilibrium MD (reverse NEMD) approach to computing thermal conductivity. This is because the usual NEMD approach is to impose a temperature gradient on the system and measure the response as the resulting heat flux. In the Muller-Plathe method, the heat flux is imposed, and the temperature gradient is the system's response.

See the *compute heat/flux* command for details on how to compute thermal conductivity in an alternate way, via the Green-Kubo formalism.

The simulation box is divided into *Nbin* layers in the *edim* direction, where the layer 1 is at the low end of that dimension and the layer *Nbin* is at the high end. Every N steps, Nswap pairs of atoms are chosen in the following manner. Only atoms in the fix group are considered. The hottest Nswap atoms in layer 1 are selected. Similarly, the coldest Nswap atoms in the "middle" layer (see below) are selected. The two sets of Nswap atoms are paired up and their velocities are exchanged. This effectively swaps their kinetic energies, assuming their masses are the same. If the masses are different, an exchange of velocities relative to center of mass motion of the 2 atoms is performed, to conserve kinetic energy. Over time, this induces a temperature gradient in the system which can be measured using commands such as the following, which writes the temperature profile (assuming z = edim) to the file tmp.profile:

```
compute   ke all ke/atom
variable  temp atom c_ke/1.5
compute   layers all chunk/atom bin/1d z lower 0.05 units reduced
fix       3 all ave/chunk 10 100 1000 layers v_temp file tmp.profile
```

Note that by default, Nswap = 1, though this can be changed by the optional *swap* keyword. Setting this parameter appropriately, in conjunction with the swap rate N, allows the heat flux to be adjusted across a wide range of values, and the kinetic energy to be exchanged in large chunks or more smoothly.

The "middle" layer for velocity swapping is defined as the *Nbin*/2 + 1 layer. Thus if *Nbin* = 20, the two swapping layers are 1 and 11. This should lead to a symmetric temperature profile since the two layers are separated by the same distance in both directions in a periodic sense. This is why *Nbin* is restricted to being an even number.

As described below, the total kinetic energy transferred by these swaps is computed by the fix and can be output. Dividing this quantity by time and the cross-sectional area of the simulation box yields a heat flux. The ratio of heat flux to the slope of the temperature profile is proportional to the thermal conductivity of the fluid, in appropriate units. See the *Muller-Plathe paper* for details.

Note: If your system is periodic in the direction of the heat flux, then the flux is going in 2 directions. This means the effective heat flux in one direction is reduced by a factor of 2. You will see this in the equations for thermal conductivity (kappa) in the Muller-Plathe paper. LAMMPS is simply tallying kinetic energy which does not account for whether or not your system is periodic; you must use the value appropriately to yield a kappa for your system.

Note: After equilibration, if the temperature gradient you observe is not linear, then you are likely swapping energy too frequently and are not in a regime of linear response. In this case you cannot accurately infer a thermal conductivity and should try increasing the Nevery parameter.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the cumulative kinetic energy transferred between the bottom and middle of the simulation box (in the *edim* direction) is stored as a scalar quantity by this fix. This quantity is zeroed when the fix is defined and accumulates thereafter, once every N steps. The units of the quantity are energy; see the *units* command for details. The scalar value calculated by this fix is "intensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.240.4 Restrictions

This fix is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Swaps conserve both momentum and kinetic energy, even if the masses of the swapped atoms are not equal. Thus you should not need to thermostat the system. If you do use a thermostat, you may want to apply it only to the non-swapped dimensions (other than *vdim*).

LAMMPS does not check, but you should not use this fix to swap the kinetic energy of atoms that are in constrained molecules, e.g. via *fix shake* or *fix rigid*. This is because application of the constraints will alter the amount of transferred momentum. You should, however, be able to use flexible molecules. See the *Zhang paper* for a discussion and results of this idea.

When running a simulation with large, massive particles or molecules in a background solvent, you may want to only exchange kinetic energy between solvent particles.

16.240.5 Related commands

fix ehex, *fix heat*, *fix ave/chunk*, *fix viscosity*, *compute heat/flux*

16.240.6 Default

The option defaults are swap = 1.

(Muller-Plathe) Muller-Plathe, J Chem Phys, 106, 6082 (1997).

(Zhang) Zhang, Lussetti, de Souza, Muller-Plathe, J Phys Chem B, 109, 15060-15067 (2005).

16.241 fix ti/spring command

16.241.1 Syntax

```
fix ID group-ID ti/spring k t_s t_eq keyword value ...
```

- ID, group-ID are documented in *fix* command
- ti/spring = style name of this fix command
- k = spring constant (force/distance units)
- t_eq = number of steps for the equilibration procedure
- t_s = number of steps for the switching procedure
- zero or more keyword/value pairs may be appended to args
- keyword = *function*

  ```
  function value = function-ID
    function-ID = ID of the switching function (1 or 2)
  ```

Example:

```
fix 1 all ti/spring 50.0 2000 1000 function 2
```

16.241.2 Description

This fix allows you to compute the free energy of crystalline solids by performing a nonequilibrium thermodynamic integration between the solid of interest and an Einstein crystal. A detailed explanation of how to use this command and choose its parameters for optimal performance and accuracy is given in the paper by *Freitas*. The paper also presents a short summary of the theory of nonequilibrium thermodynamic integration.

The thermodynamic integration procedure is performed by rescaling the force on each atom. Given an atomic configuration the force (F) on each atom is given by

$$F = (1 - \lambda)\, F_{\text{solid}} + \lambda F_{\text{harm}}$$

where F_solid is the force that acts on an atom due to an interatomic potential (*e.g.* EAM potential), F_harm is the force due to the Einstein crystal harmonic spring, and lambda is the coupling parameter of the thermodynamic integration. An Einstein crystal is a solid where each atom is attached to its equilibrium position by a harmonic spring with spring

constant *k*. With this fix a spring force is applied independently to each atom in the group defined by the fix to tether it to its initial position. The initial position of each atom is its position at the time the fix command was issued.

The fix acts as follows: during the first *t_eq* steps after the fix is defined the value of lambda is zero. This is the period to equilibrate the system in the lambda = 0 state. After this the value of lambda changes dynamically during the simulation from 0 to 1 according to the function defined using the keyword *function* (described below), this switching from lambda from 0 to 1 is done in *t_s* steps. Then comes the second equilibration period of *t_eq* to equilibrate the system in the lambda = 1 state. After that, the switching back to the lambda = 0 state is made using *t_s* timesteps and following the same switching function. After this period the value of lambda is kept equal to zero and the fix has no other effect on the dynamics of the system.

The processes described above is known as nonequilibrium thermodynamic integration and is has been shown (*Freitas*) to present a much superior efficiency when compared to standard equilibrium methods. The reason why the switching it is made in both directions (potential to Einstein crystal and back) is to eliminate the dissipated heat due to the nonequilibrium process. Further details about nonequilibrium thermodynamic integration and its implementation in LAMMPS is available in *Freitas*.

The *function* keyword allows the use of two different lambda paths. Option *1* results in a constant rate of change of lambda with time:

$$\lambda(\tau) = \tau$$

where tau is the scaled time variable *t/t_s*. The option *2* performs the lambda switching at a rate defined by the following switching function

$$\lambda(\tau) = \tau^5 \left(70\tau^4 - 315\tau^3 + 540\tau^2 - 420\tau + 126\right)$$

This function has zero slope as lambda approaches its extreme values (0 and 1), according to *de Koning* this results in smaller fluctuations on the integral to be computed on the thermodynamic integration. The use of option *2* is recommended since it results in better accuracy and less dissipation without any increase in computational resources cost.

Note: As described in *Freitas*, it is important to keep the center-of-mass fixed during the thermodynamic integration. A nonzero total velocity will result in divergences during the integration due to the fact that the atoms are 'attached' to their equilibrium positions by the Einstein crystal. Check the option *zero* of *fix langevin* and *velocity*. The use of the Nose-Hoover thermostat (*fix nvt*) is *NOT* recommended due to its well documented issues with the canonical sampling of harmonic degrees of freedom (notice that the *chain* option will *NOT* solve this problem). The Langevin thermostat (*fix langevin*) correctly thermostats the system and we advise its usage with ti/spring command.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the original coordinates of tethered atoms to *binary restart files*, so that the spring effect will be the same in a restarted simulation. See the *read restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The *fix modify energy* option is supported by this fix to add the energy stored in the per-atom springs to the system's potential energy as part of *thermodynamic output*.

This fix computes a global scalar and a global vector quantities which can be accessed by various *output commands*. The scalar is an energy which is the sum of the spring energy for each atom, where the per-atom energy is 0.5 * k * r^2. The vector has 2 positions, the first one is the coupling parameter lambda and the second one is the time derivative of lambda. The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command.

Note: If you want the per-atom spring energy to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the *fix modify energy* option for this fix.

16.241.3 Related commands

fix spring, *fix adapt*

16.241.4 Restrictions

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.241.5 Default

The keyword default is function = 1.

(Freitas) Freitas, Asta, and de Koning, Computational Materials Science, 112, 333 (2016).

(de Koning) de Koning and Antonelli, Phys Rev E, 53, 465 (1996).

16.242 fix tmd command

16.242.1 Syntax

```
fix ID group-ID tmd rho_final file1 N file2
```

- ID, group-ID are documented in *fix* command
- tmd = style name of this fix command
- rho_final = desired value of rho at the end of the run (distance units)
- file1 = filename to read target structure from
- N = dump TMD statistics every this many timesteps, 0 = no dump
- file2 = filename to write TMD statistics to (only needed if N > 0)

16.242.2 Examples

```
fix 1 all nve
fix 2 tmdatoms tmd 1.0 target_file 100 tmd_dump_file
```

16.242.3 Description

Perform targeted molecular dynamics (TMD) on a group of atoms. A holonomic constraint is used to force the atoms to move towards (or away from) the target configuration. The parameter "rho" is monotonically decreased (or increased) from its initial value to rho_final at the end of the run.

Rho has distance units and is a measure of the root-mean-squared distance (RMSD) between the current configuration of the atoms in the group and the target coordinates listed in file1. Thus a value of rho_final = 0.0 means move the atoms all the way to the final structure during the course of the run.

The target file1 can be ASCII text or a gzipped text file (detected by a .gz suffix). The format of the target file1 is as follows:

```
0.0 25.0 xlo xhi
0.0 25.0 ylo yhi
0.0 25.0 zlo zhi
125     24.97311   1.69005     23.46956 0 0 -1
126     1.94691    2.79640     1.92799  1 0 0
127     0.15906    3.46099     0.79121  1 0 0
...
```

The first 3 lines may or may not be needed, depending on the format of the atoms to follow. If image flags are included with the atoms, the 1st 3 lo/hi lines must appear in the file. If image flags are not included, the 1st 3 lines should not appear. The 3 lines contain the simulation box dimensions for the atom coordinates, in the same format as in a LAMMPS data file (see the *read_data* command).

The remaining lines each contain an atom ID and its target x,y,z coordinates. The atom lines (all or none of them) can optionally be followed by 3 integer values: nx,ny,nz. For periodic dimensions, they specify which image of the box the atom is considered to be in, i.e. a value of N (positive or negative) means add N times the box length to the coordinate to get the true value.

The atom lines can be listed in any order, but every atom in the group must be listed in the file. Atoms not in the fix group may also be listed; they will be ignored.

TMD statistics are written to file2 every N timesteps, unless N is specified as 0, which means no statistics.

The atoms in the fix tmd group should be integrated (via a fix nve, nvt, npt) along with other atoms in the system.

Restarts can be used with a fix tmd command. For example, imagine a 10000 timestep run with a rho_initial = 11 and a rho_final = 1. If a restart file was written after 2000 time steps, then the configuration in the file would have a rho value of 9. A new 8000 time step run could be performed with the same rho_final = 1 to complete the conformational change at the same transition rate. Note that for restarted runs, the name of the TMD statistics file should be changed to prevent it being overwritten.

For more information about TMD, see *(Schlitter1)* and *(Schlitter2)*.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*.

This fix can ramp its rho parameter over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during *energy minimization*.

16.242.4 Restrictions

All TMD fixes must be listed in the input script after all integrator fixes (nve, nvt, npt) are applied. This ensures that atoms are moved before their positions are corrected to comply with the constraint.

Atoms that have a TMD fix applied should not be part of a group to which a SHAKE fix is applied. This is because LAMMPS assumes there are not multiple competing holonomic constraints applied to the same atoms.

To read gzipped target files, you must compile LAMMPS with the -DLAMMPS_GZIP option. See the *Build settings* doc page for details.

Related commands: none

Default: none

(Schlitter1) Schlitter, Swegat, Mulders, "Distance-type reaction coordinates for modelling activated processes", J Molecular Modeling, 7, 171-177 (2001).

(Schlitter2) Schlitter and Klahn, "The free energy of a reaction coordinate at multiple constraints: a concise formulation", Molecular Physics, 101, 3439-3443 (2003).

16.243 fix ttm command

16.244 fix ttm/mod command

16.244.1 Syntax

```
fix ID group-ID ttm seed C_e rho_e kappa_e gamma_p gamma_s v_0 Nx Ny Nz T_infile N T_
↪outfile
fix ID group-ID ttm/mod seed init_file Nx Ny Nz T_infile N T_outfile
```

- ID, group-ID are documented in *fix* command
- style = *ttm* or *ttm_mod*
- seed = random number seed to use for white noise (positive integer)
- remaining arguments for fix ttm:

```
C_e  = electronic specific heat (energy/(electron*temperature) units)
rho_e = electronic density (electrons/volume units)
kappa_e = electronic thermal conductivity (energy/(time*distance*temperature)␣
↪units)
gamma_p = friction coefficient due to electron-ion interactions (mass/
↪time units)
gamma_s = friction coefficient due to electronic stopping (mass/time␣
↪units)
v_0 = electronic stopping critical velocity (velocity units)
Nx = number of thermal solve grid points in the x-direction (positive␣
↪integer)
Ny = number of thermal solve grid points in the y-direction (positive␣
↪integer)
Nz = number of thermal solve grid points in the z-direction (positive␣
↪integer)
T_infile = filename to read initial electronic temperature from
```

```
N = dump TTM temperatures every this many timesteps, 0 = no dump
T_outfile = filename to write TTM temperatures to (only needed if N > 0)
```

- remaining arguments for fix ttm/mod:

```
init_file = file with the parameters to TTM
Nx = number of thermal solve grid points in the x-direction (positive integer)
Ny = number of thermal solve grid points in the y-direction (positive integer)
Nz = number of thermal solve grid points in the z-direction (positive integer)
T_infile = filename to read initial electronic temperature from
N = dump TTM temperatures every this many timesteps, 0 = no dump
T_outfile = filename to write TTM temperatures to (only needed if N > 0)
```

16.244.2 Examples

```
fix 2 all ttm 699489 1.0 1.0 10 0.1 0.0 2.0 1 12 1 initialTs 1000 T.out
fix 2 all ttm 123456 1.0 1.0 1.0 1.0 1.0 5.0 5 5 5 Te.in 1 Te.out
fix 2 all ttm/mod 34277 parameters.txt 5 5 5 T_init 10 T_out
```

16.244.3 Description

Use a two-temperature model (TTM) to represent heat transfer through and between electronic and atomic subsystems. LAMMPS models the atomic subsystem as usual with a molecular dynamics model and the classical force field specified by the user, but the electronic subsystem is modeled as a continuum, or a background "gas", on a regular grid. Energy can be transferred spatially within the grid representing the electrons. Energy can also be transferred between the electronic and the atomic subsystems. The algorithm underlying this fix was derived by D. M. Duffy and A. M. Rutherford and is discussed in two J Physics: Condensed Matter papers: *(Duffy)* and *(Rutherford)*. They used this algorithm in cascade simulations where a primary knock-on atom (PKA) was initialized with a high velocity to simulate a radiation event.

The description in this sub-section applies to both fix ttm and fix ttm/mod. Fix ttm/mod adds options to account for external heat sources (e.g. at a surface) and for specifying parameters that allow the electronic heat capacity to depend strongly on electronic temperature. It is more expensive computationally than fix ttm because it treats the thermal diffusion equation as non-linear. More details on fix ttm/mod are given below.

Heat transfer between the electronic and atomic subsystems is carried out via an inhomogeneous Langevin thermostat. This thermostat differs from the regular Langevin thermostat (*fix langevin*) in three important ways. First, the Langevin thermostat is applied uniformly to all atoms in the user-specified group for a single target temperature, whereas the TTM fix applies Langevin thermostatting locally to atoms within the volumes represented by the user-specified grid points with a target temperature specific to that grid point. Second, the Langevin thermostat couples the temperature of the atoms to an infinite heat reservoir, whereas the heat reservoir for fix TTM is finite and represents the local electrons. Third, the TTM fix allows users to specify not just one friction coefficient, but rather two independent friction coefficients: one for the electron-ion interactions (*gamma_p*), and one for electron stopping (*gamma_s*).

When the friction coefficient due to electron stopping, *gamma_s*, is non-zero, electron stopping effects are included for atoms moving faster than the electron stopping critical velocity, *v_0*. For further details about this algorithm, see *(Duffy)* and *(Rutherford)*.

Energy transport within the electronic subsystem is solved according to the heat diffusion equation with added source terms for heat transfer between the subsystems:

$$C_e \rho_e \frac{\partial T_e}{\partial t} = \bigtriangledown(\kappa_e \bigtriangledown T_e) - g_p(T_e - T_a) + g_s T'_a$$

where C_e is the specific heat, rho_e is the density, kappa_e is the thermal conductivity, T is temperature, the "e" and "a" subscripts represent electronic and atomic subsystems respectively, g_p is the coupling constant for the electron-ion

interaction, and g_s is the electron stopping coupling parameter. C_e, rho_e, and kappa_e are specified as parameters to the fix. The other quantities are derived. The form of the heat diffusion equation used here is almost the same as that in equation 6 of *(Duffy)*, with the exception that the electronic density is explicitly represented, rather than being part of the specific heat parameter.

Currently, fix ttm assumes that none of the user-supplied parameters will vary with temperature. Note that *(Duffy)* used a tanh() functional form for the temperature dependence of the electronic specific heat, but ignored temperature dependencies of any of the other parameters. See more discussion below for fix ttm/mod.

These fixes require use of periodic boundary conditions and a 3D simulation. Periodic boundary conditions are also used in the heat equation solve for the electronic subsystem. This varies from the approach of *(Rutherford)* where the atomic subsystem was embedded within a larger continuum representation of the electronic subsystem.

The initial electronic temperature input file, *T_infile*, is a text file LAMMPS reads in with no header and with four numeric columns (ix,iy,iz,Temp) and with a number of rows equal to the number of user-specified grid points (Nx by Ny by Nz). The ix,iy,iz are node indices from 0 to nxnodes-1, etc. For example, the initial electronic temperatures on a 1 by 2 by 3 grid could be specified in a *T_infile* as follows:

```
0 0 0 1.0
0 0 1 1.0
0 0 2 1.0
0 1 0 2.0
0 1 1 2.0
0 1 2 2.0
```

where the electronic temperatures along the y=0 plane have been set to 1.0, and the electronic temperatures along the y=1 plane have been set to 2.0. The order of lines in this file is no important. If all the nodal values are not specified, LAMMPS will generate an error.

The temperature output file, *T_oufile*, is created and written by this fix. Temperatures for both the electronic and atomic subsystems at every node and every N timesteps are output. If N is specified as zero, no output is generated, and no output filename is needed. The format of the output is as follows. One long line is written every output timestep. The timestep itself is given in the first column. The next Nx*Ny*Nz columns contain the temperatures for the atomic subsystem, and the final Nx*Ny*Nz columns contain the temperatures for the electronic subsystem. The ordering of the Nx*Ny*Nz columns is with the z index varying fastest, y the next fastest, and x the slowest.

These fixes do not change the coordinates of their atoms; they only scales their velocities. Thus a time integration fix (e.g. *fix nve*) should still be used to time integrate the affected atoms. The fixes should not normally be used on atoms that have their temperature controlled by another fix - e.g. *fix nvt* or *fix langevin*.

Note: The current implementations of these fixes create a copy of the electron grid that overlays the entire simulation domain, for each processor. Values on the grid are summed across all processors. Thus you should insure that this grid is not too large, else your simulation could incur high memory and communication costs.

Additional details for fix ttm/mod

Fix ttm/mod uses the heat diffusion equation with possible external heat sources (e.g. laser heating in ablation simulations):

$$C_e \rho_e \frac{\partial T_e}{\partial t} = \bigtriangledown(\kappa_e \bigtriangledown T_e) - g_p(T_e - T_a) + g_s T'_a + \theta(x - x_{surface}) I_0 \exp(-x/l_{skin})$$

where theta is the Heaviside step function, I_0 is the (absorbed) laser pulse intensity for ablation simulations, l_skin is the depth of skin-layer, and all other designations have the same meaning as in the former equation. The duration of the pulse is set by the parameter *tau* in the *init_file*.

Fix ttm/mod also allows users to specify the dependencies of C_e and kappa_e on the electronic temperature. The specific heat is expressed as

$$C_e = C_0 + (a_0 + a_1 X + a_2 X^2 + a_3 X^3 + a_4 X^4) \exp(-(AX)^2)$$

where *X* = T_e/1000, and the thermal conductivity is defined as kappa_e = D_e*rho_e*C_e, where D_e is the thermal diffusion coefficient.

Electronic pressure effects are included in the TTM model to account for the blast force acting on ions because of electronic pressure gradient (see *(Chen)*, *(Norman)*). The total force acting on an ion is:

$$\vec{F}_i = -\partial U/\partial \vec{r}_i + \vec{F}_{langevin} - \nabla P_e/n_{ion}$$

where F_langevin is a force from Langevin thermostat simulating electron-phonon coupling, and nabla P_e/n_ion is the electron blast force.

The electronic pressure is taken to be P_e = B*rho_e*C_e*T_e

The current fix ttm/mod implementation allows TTM simulations with a vacuum. The vacuum region is defined as the grid cells with zero electronic temperature. The numerical scheme does not allow energy exchange with such cells. Since the material can expand to previously unoccupied region in some simulations, the vacuum border can be allowed to move. It is controlled by the *surface_movement* parameter in the *init_file*. If it is set to 1, then "vacuum" cells can be changed to "electron-filled" cells with the temperature *T_e_min* if atoms move into them (currently only implemented for the case of 1-dimensional motion of flat surface normal to the X axis). The initial borders of vacuum can be set in the *init_file* via *lsurface* and *rsurface* parameters. In this case, electronic pressure gradient is calculated as

$$\nabla_x P_e = \left[\frac{C_e T_e(x) \lambda}{(x+\lambda)^2} + \frac{x}{x+\lambda} \frac{(C_e T_e)_{x+\Delta x} - (C_e T_e)_x}{\Delta x} \right]$$

where lambda is the electron mean free path (see *(Norman)*, *(Pisarev)*)

The fix ttm/mod parameter file *init_file* has the following syntax/ Every line with the odd number is considered as a comment and ignored. The lines with the even numbers are treated as follows:

```
a_0, energy/(temperature*electron) units
a_1, energy/(temperature^2*electron) units
a_2, energy/(temperature^3*electron) units
a_3, energy/(temperature^4*electron) units
a_4, energy/(temperature^5*electron) units
C_0, energy/(temperature*electron) units
A, 1/temperature units
rho_e, electrons/volume units
D_e, length^2/time units
gamma_p, mass/time units
gamma_s, mass/time units
v_0, length/time units
I_0, energy/(time*length^2) units
lsurface, electron grid units (positive integer)
rsurface, electron grid units (positive integer)
l_skin, length units
tau, time units
B, dimensionless
lambda, length units
n_ion, ions/volume units
surface_movement: 0 to disable tracking of surface motion, 1 to enable
T_e_min, temperature units
```

Restart, fix_modify, output, run start/stop, minimize info:

These fixes write the state of the electronic subsystem and the energy exchange between the subsystems to *binary restart files*. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

Because the state of the random number generator is not saved in the restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior.

None of the *fix_modify* options are relevant to these fixes.

Both fixes compute 2 output quantities stored in a vector of length 2, which can be accessed by various *output commands*. The first quantity is the total energy of the electronic subsystem. The second quantity is the energy transferred from the electronic to the atomic subsystem on that timestep. Note that the velocity verlet integrator applies the fix ttm forces to the atomic subsystem as two half-step velocity updates: one on the current timestep and one on the subsequent timestep. Consequently, the change in the atomic subsystem energy is lagged by half a timestep relative to the change in the electronic subsystem energy. As a result of this, users may notice slight fluctuations in the sum of the atomic and electronic subsystem energies reported at the end of the timestep.

The vector values calculated are "extensive".

No parameter of the fixes can be used with the *start/stop* keywords of the *run* command. The fixes are not invoked during *energy minimization*.

16.244.4 Restrictions

Fix *ttm* is part of the MISC package. It is only enabled if LAMMPS was built with that package. Fix *ttm/mod* is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

These fixes can only be used for 3d simulations and orthogonal simulation boxes. You must also use periodic *boundary* conditions.

16.244.5 Related commands

fix langevin, *fix dt/reset*

Default: none

(Duffy) D M Duffy and A M Rutherford, J. Phys.: Condens. Matter, 19, 016207-016218 (2007).

(Rutherford) A M Rutherford and D M Duffy, J. Phys.: Condens. Matter, 19, 496201-496210 (2007).

(Chen) J Chen, D Tzou and J Beraun, Int. J. Heat Mass Transfer, 49, 307-316 (2006).

(Norman) G E Norman, S V Starikov, V V Stegailov et al., Contrib. Plasma Phys., 53, 129-139 (2013).

(Pisarev) V V Pisarev and S V Starikov, J. Phys.: Condens. Matter, 26, 475401 (2014).

16.245 fix tune/kspace command

16.245.1 Syntax

```
fix ID group-ID tune/kspace N
```

- ID, group-ID are documented in *fix* command
- tune/kspace = style name of this fix command
- N = invoke this fix every N steps

16.245.2 Examples

```
fix 2 all tune/kspace 100
```

16.245.3 Description

This fix tests each kspace style (Ewald, PPPM, and MSM), and automatically selects the fastest style to use for the remainder of the run. If the fastest style is Ewald or PPPM, the fix also adjusts the Coulombic cutoff towards optimal speed. Future versions of this fix will automatically select other kspace parameters to use for maximum simulation speed. The kspace parameters may include the style, cutoff, grid points in each direction, order, Ewald parameter, MSM parallelization cut-point, MPI tasks to use, etc.

The rationale for this fix is to provide the user with as-fast-as-possible simulations that include long-range electrostatics (kspace) while meeting the user-prescribed accuracy requirement. A simple heuristic could never capture the optimal combination of parameters for every possible run-time scenario. But by performing short tests of various kspace parameter sets, this fix allows parameters to be tailored specifically to the user's machine, MPI ranks, use of threading or accelerators, the simulated system, and the simulation details. In addition, it is possible that parameters could be evolved with the simulation on-the-fly, which is useful for systems that are dynamically evolving (e.g. changes in box size/shape or number of particles).

When this fix is invoked, LAMMPS will perform short timed tests of various parameter sets to determine the optimal parameters. Tests are performed on-the-fly, with a new test initialized every N steps. N should be chosen large enough so that adequate CPU time lapses between tests, thereby providing statistically significant timings. But N should not be chosen to be so large that an unfortunate parameter set test takes an inordinate amount of wall time to complete. An N of 100 for most problems seems reasonable. Once an optimal parameter set is found, that set is used for the remainder of the run.

This fix uses heuristics to guide it's selection of parameter sets to test, but the actual timed results will be used to decide which set to use in the simulation.

It is not necessary to discard trajectories produced using sub-optimal parameter sets, or a mix of various parameter sets, since the user-prescribed accuracy will have been maintained throughout. However, some users may prefer to use this fix only to discover the optimal parameter set for a given setup that can then be used on subsequent production runs.

This fix starts with kspace parameters that are set by the user with the *kspace_style* and *kspace_modify* commands. The prescribed accuracy will be maintained by this fix throughout the simulation.

None of the *fix_modify* options are relevant to this fix.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.245.4 Restrictions

This fix is part of the KSPACE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Do not set "neigh_modify once yes" or else this fix will never be called. Reneighboring is required.

This fix is not compatible with a hybrid pair style, long-range dispersion, TIP4P water support, or long-range point dipole support.

16.245.5 Related commands

kspace_style, *boundary kspace_modify*, *pair_style lj/cut/coul/long*, *pair_style lj/charmm/coul/long*, *pair_style lj/long*, *pair_style lj/long/coul/long*, *pair_style buck/coul/long*

16.245.6 Default

16.246 fix vector command

16.246.1 Syntax

```
fix ID group-ID vector Nevery value1 value2 ...
```

- ID, group-ID are documented in *fix* command
- vector = style name of this fix command
- Nevery = use input values every this many timesteps
- one or more input values can be listed
- value = c_ID, c_ID[N], f_ID, f_ID[N], v_name

```
c_ID = global scalar calculated by a compute with ID
c_ID[I] = Ith component of global vector calculated by a compute with ID
f_ID = global scalar calculated by a fix with ID
f_ID[I] = Ith component of global vector calculated by a fix with ID
v_name = value calculated by an equal-style variable with name
v_name[I] = Ith component of vector-style variable with name
```

16.246.2 Examples

```
fix 1 all vector 100 c_myTemp
fix 1 all vector 5 c_myTemp v_integral
```

16.246.3 Description

Use one or more global values as inputs every few timesteps, and simply store them. For a single specified value, the values are stored as a global vector of growing length. For multiple specified values, they are stored as rows in a global array, whose number of rows is growing. The resulting vector or array can be used by other *output commands*.

One way to to use this command is to accumulate a vector that is time-integrated using the *variable trap()* function. For example the velocity auto-correlation function (VACF) can be time-integrated, to yield a diffusion coefficient, as follows:

```
compute         2 all vacf
fix             5 all vector 1 c_2[4]
variable        diff equal dt*trap(f_5)
thermo_style    custom step v_diff
```

The group specified with this command is ignored. However, note that specified values may represent calculations performed by computes and fixes which store their own "group" definitions.

Each listed value can be the result of a *compute* or *fix* or the evaluation of an equal-style or vector-style *variable*. In each case, the compute, fix, or variable must produce a global quantity, not a per-atom or local quantity. And the global quantity must be a scalar, not a vector or array.

Computes that produce global quantities are those which do not have the word *atom* in their style name. Only a few *fixes* produce global quantities. See the doc pages for individual fixes for info on which ones produce such values. *Variables* of style *equal* or *vector* are the only ones that can be used with this fix. Variables of style *atom* cannot be used, since they produce per-atom values.

The *Nevery* argument specifies on what timesteps the input values will be used in order to be stored. Only timesteps that are a multiple of *Nevery*, including timestep 0, will contribute values.

Note that if you perform multiple runs, using the "pre no" option of the *run* command to avoid initialization on subsequent runs, then you need to use the *stop* keyword with the first *run* command with a timestep value that encompasses all the runs. This is so that the vector or array stored by this fix can be allocated to a sufficient size.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If no bracketed term is appended, the global scalar calculated by the compute is used. If a bracketed term is appended, the Ith element of the global vector calculated by the compute is used.

Note that there is a *compute reduce* command which can sum per-atom quantities into a global scalar or vector which can thus be accessed by fix vector. Or it can be a compute defined not in your input script, but by *thermodynamic output* or other fixes such as *fix nvt* or *fix temp/rescale*. See the doc pages for these commands which give the IDs of these computes. Users can also write code for their own compute styles and *add them to LAMMPS*.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If no bracketed term is appended, the global scalar calculated by the fix is used. If a bracketed term is appended, the Ith element of the global vector calculated by the fix is used.

Note that some fixes only produce their values on certain timesteps, which must be compatible with *Nevery*, else an error will result. Users can also write code for their own fix styles and *add them to LAMMPS*.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. An equal-style or vector-style variable can be referenced; the latter requires a bracketed term to specify the Ith element of the vector calculated by the variable. See the *variable* command for details. Note that variables of style *equal* and *vector* define a formula which can reference individual atom properties or thermodynamic keywords, or they can invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of specifying quantities to be stored by fix vector.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix produces a global vector or global array which can be accessed by various *output commands*. The values can only be accessed on timesteps that are multiples of *Nevery*.

A vector is produced if only a single input value is specified. An array is produced if multiple input values are specified. The length of the vector or the number of rows in the array grows by 1 every *Nevery* timesteps.

If the fix produces a vector, then the entire vector will be either "intensive" or "extensive", depending on whether the values stored in the vector are "intensive" or "extensive". If the fix produces an array, then all elements in the array must be the same, either "intensive" or "extensive". If a compute or fix provides the value stored, then the compute or fix determines whether the value is intensive or extensive; see the doc page for that compute or fix for further info. Values produced by a variable are treated as intensive.

This fix can allocate storage for stored values accumulated over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this. If using the *run pre no* command option, this is required to allow the fix to allocate sufficient storage for stored values.

This fix is not invoked during *energy minimization*.

16.246.4 Restrictions

none

16.246.5 Related commands

compute, *variable*

Default: none

16.247 fix viscosity command

16.247.1 Syntax

```
fix ID group-ID viscosity N vdim pdim Nbin keyword value ...
```

- ID, group-ID are documented in *fix* command
- viscosity = style name of this fix command
- N = perform momentum exchange every N steps
- vdim = *x* or *y* or *z* = which momentum component to exchange
- pdim = *x* or *y* or *z* = direction of momentum transfer
- Nbin = # of layers in pdim direction (must be even number)
- zero or more keyword/value pairs may be appended
- keyword = *swap* or *target*

  ```
  swap value = Nswap = number of swaps to perform every N steps
  vtarget value = V or INF = target velocity of swap partners (velocity␣
  ↪units)
  ```

16.247.2 Examples

```
fix 1 all viscosity 100 x z 20
fix 1 all viscosity 50 x z 20 swap 2 vtarget 1.5
```

16.247.3 Description

Use the Muller-Plathe algorithm described in *this paper* to exchange momenta between two particles in different regions of the simulation box every N steps. This induces a shear velocity profile in the system. As described below this enables a viscosity of the fluid to be calculated. This algorithm is sometimes called a reverse non-equilibrium MD (reverse NEMD) approach to computing viscosity. This is because the usual NEMD approach is to impose a shear velocity profile on the system and measure the response via an off-diagonal component of the stress tensor, which is proportional to the momentum flux. In the Muller-Plathe method, the momentum flux is imposed, and the shear velocity profile is the system's response.

The simulation box is divided into *Nbin* layers in the *pdim* direction, where the layer 1 is at the low end of that dimension and the layer *Nbin* is at the high end. Every N steps, Nswap pairs of atoms are chosen in the following manner. Only atoms in the fix group are considered. Nswap atoms in layer 1 with positive velocity components in the *vdim* direction closest to the target value *V* are selected. Similarly, Nswap atoms in the "middle" layer (see below) with negative velocity components in the *vdim* direction closest to the negative of the target value *V* are selected. The two sets of Nswap atoms are paired up and their *vdim* momenta components are swapped within each pair. This resets their velocities, typically in opposite directions. Over time, this induces a shear velocity profile in the system which can be measured using commands such as the following, which writes the profile to the file tmp.profile:

```
compute layers all chunk/atom bin/1d z lower 0.05 units reduced
fix f1 all ave/chunk 100 10 1000 layers vx file tmp.profile
```

Note that by default, Nswap = 1 and vtarget = INF, though this can be changed by the optional *swap* and *vtarget* keywords. When vtarget = INF, one or more atoms with the most positive and negative velocity components are selected. Setting these parameters appropriately, in conjunction with the swap rate N, allows the momentum flux rate to be adjusted across a wide range of values, and the momenta to be exchanged in large chunks or more smoothly.

The "middle" layer for momenta swapping is defined as the *Nbin*/2 + 1 layer. Thus if *Nbin* = 20, the two swapping layers are 1 and 11. This should lead to a symmetric velocity profile since the two layers are separated by the same distance in both directions in a periodic sense. This is why *Nbin* is restricted to being an even number.

As described below, the total momentum transferred by these velocity swaps is computed by the fix and can be output. Dividing this quantity by time and the cross-sectional area of the simulation box yields a momentum flux. The ratio of momentum flux to the slope of the shear velocity profile is proportional to the viscosity of the fluid, in appropriate units. See the *Muller-Plathe paper* for details.

Note: If your system is periodic in the direction of the momentum flux, then the flux is going in 2 directions. This means the effective momentum flux in one direction is reduced by a factor of 2. You will see this in the equations for viscosity in the Muller-Plathe paper. LAMMPS is simply tallying momentum which does not account for whether or not your system is periodic; you must use the value appropriately to yield a viscosity for your system.

Note: After equilibration, if the velocity profile you observe is not linear, then you are likely swapping momentum too frequently and are not in a regime of linear response. In this case you cannot accurately infer a viscosity and should try increasing the Nevery parameter.

An alternative method for calculating a viscosity is to run a NEMD simulation, as described on the *Howto nemd* doc page. NEMD simulations deform the simulation box via the *fix deform* command. Thus they cannot be run

on a charged system using a *PPPM solver* since PPPM does not currently support non-orthogonal boxes. Using fix viscosity keeps the box orthogonal; thus it does not suffer from this limitation.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix computes a global scalar which can be accessed by various *output commands*. The scalar is the cumulative momentum transferred between the bottom and middle of the simulation box (in the *pdim* direction) is stored as a scalar quantity by this fix. This quantity is zeroed when the fix is defined and accumulates thereafter, once every N steps. The units of the quantity are momentum = mass*velocity. The scalar value calculated by this fix is "intensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.247.4 Restrictions

This fix is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Swaps conserve both momentum and kinetic energy, even if the masses of the swapped atoms are not equal. Thus you should not need to thermostat the system. If you do use a thermostat, you may want to apply it only to the non-swapped dimensions (other than *vdim*).

LAMMPS does not check, but you should not use this fix to swap velocities of atoms that are in constrained molecules, e.g. via *fix shake* or *fix rigid*. This is because application of the constraints will alter the amount of transferred momentum. You should, however, be able to use flexible molecules. See the *Maginn paper* for an example of using this algorithm in a computation of alcohol molecule properties.

When running a simulation with large, massive particles or molecules in a background solvent, you may want to only exchange momenta between solvent particles.

16.247.5 Related commands

fix ave/chunk, *fix thermal/conductivity*

16.247.6 Default

The option defaults are swap = 1 and vtarget = INF.

(Muller-Plathe) Muller-Plathe, Phys Rev E, 59, 4894-4898 (1999).

(Maginn) Kelkar, Rafferty, Maginn, Siepmann, Fluid Phase Equilibria, 260, 218-231 (2007).

16.248 fix viscous command

16.248.1 Syntax

```
fix ID group-ID viscous gamma keyword values ...
```

- ID, group-ID are documented in *fix* command
- viscous = style name of this fix command

- gamma = damping coefficient (force/velocity units)
- zero or more keyword/value pairs may be appended

```
keyword = scale
  scale values = type ratio
    type = atom type (1-N)
    ratio = factor to scale the damping coefficient by
```

16.248.2 Examples

```
fix 1 flow viscous 0.1
fix 1 damp viscous 0.5 scale 3 2.5
```

16.248.3 Description

Add a viscous damping force to atoms in the group that is proportional to the velocity of the atom. The added force can be thought of as a frictional interaction with implicit solvent, i.e. the no-slip Stokes drag on a spherical particle. In granular simulations this can be useful for draining the kinetic energy from the system in a controlled fashion. If used without additional thermostatting (to add kinetic energy to the system), it has the effect of slowly (or rapidly) freezing the system; hence it can also be used as a simple energy minimization technique.

The damping force F_i is given by $F_i = -\gamma v_i$. The larger the coefficient, the faster the kinetic energy is reduced. If the optional keyword *scale* is used, γ can scaled up or down by the specified factor for atoms of that type. It can be used multiple times to adjust γ for several atom types.

Note: You should specify gamma in force/velocity units. This is not the same as mass/time units, at least for some of the LAMMPS *units* options like "real" or "metal" that are not self-consistent.

In a Brownian dynamics context, $\gamma = \frac{k_B T}{D}$, where k_B = Boltzmann's constant, T = temperature, and D = particle diffusion coefficient. D can be written as $\frac{k_B T}{3\pi\eta d}$, where η = dynamic viscosity of the frictional fluid and d = diameter of particle. This means $\gamma = 3\pi\eta d$, and thus is proportional to the viscosity of the fluid and the particle diameter.

In the current implementation, rather than have the user specify a viscosity, γ is specified directly in force/velocity units. If needed, γ can be adjusted for atoms of different sizes (i.e. σ) by using the *scale* keyword.

Note that Brownian dynamics models also typically include a randomized force term to thermostat the system at a chosen temperature. The *fix langevin* command does this. It has the same viscous damping term as fix viscous and adds a random force to each atom. The random force term is proportional to the square root of the chosen thermostatting temperature. Thus if you use fix langevin with a target $T = 0$, its random force term is zero, and you are essentially performing the same operation as fix viscous. Also note that the gamma of fix viscous is related to the damping parameter of *fix langevin*, however the former is specified in units of force/velocity and the latter in units of time, so that it can more easily be used as a thermostat.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The *fix_modify* *respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix is modifying forces. Default is the outermost level.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command. This fix should only be used with damped dynamics minimizers that allow for non-conservative forces. See the *min_style* command for details.

16.248.4 Restrictions

none

16.248.5 Related commands

fix langevin

Default: none

16.249 fix wall/lj93 command

16.250 fix wall/lj93/kk command

16.251 fix wall/lj126 command

16.252 fix wall/lj1043 command

16.253 fix wall/colloid command

16.254 fix wall/harmonic command

16.255 fix wall/morse command

16.255.1 Syntax

```
fix ID group-ID style face args ... keyword value ...
```

- ID, group-ID are documented in *fix* command
- style = *wall/lj93* or *wall/lj126* or *wall/lj1043* or *wall/colloid* or *wall/harmonic* or *wall/morse*
- one or more face/arg pairs may be appended
- face = *xlo* or *xhi* or *ylo* or *yhi* or *zlo* or *zhi*
- args for styles *lj93* or *lj126* or *lj1043* or *colloid* or *harmonic*

```
args = coord epsilon sigma cutoff
coord = position of wall = EDGE or constant or variable
  EDGE = current lo or hi edge of simulation box
  constant = number like 0.0 or -30.0 (distance units)
  variable = equal-style variable like v_x or v_wiggle
```

```
epsilon = strength factor for wall-particle interaction (energy or energy/
↪distance^2 units)
  epsilon can be a variable (see below)
sigma = size factor for wall-particle interaction (distance units)
  sigma can be a variable (see below)
cutoff = distance from wall at which wall-particle interaction is cut off␣
↪(distance units)
```

- args for style *morse*

```
args = coord D_0 alpha r_0 cutoff
coord = position of wall = EDGE or constant or variable
  EDGE = current lo or hi edge of simulation box
  constant = number like 0.0 or -30.0 (distance units)
  variable = equal-style variable like v_x or v_wiggle
D_0 = depth of the potential (energy units)
  D_0 can be a variable (see below)
alpha = width factor for wall-particle interaction (1/distance units)
  alpha can be a variable (see below)
r_0 = distance of the potential minimum from the face of region (distance␣
↪units)
  r_0 can be a variable (see below)
cutoff = distance from wall at which wall-particle interaction is cut off␣
↪(distance units)
```

- zero or more keyword/value pairs may be appended
- keyword = *units* or *fld*

```
units value = lattice or box
  lattice = the wall position is defined in lattice units
  box = the wall position is defined in simulation box units
fld value = yes or no
  yes = invoke the wall constraint to be compatible with implicit FLD
  no = invoke the wall constraint in the normal way
pbc value = yes or no
  yes = allow periodic boundary in a wall dimension
  no = require non-perioidic boundaries in any wall dimension
```

16.255.2 Examples

```
fix wallhi all wall/lj93 xlo -1.0 1.0 1.0 2.5 units box
fix wallhi all wall/lj93 xhi EDGE 1.0 1.0 2.5
fix wallhi all wall/morse xhi EDGE 1.0 1.0 1.0 2.5 units box
fix wallhi all wall/lj126 v_wiggle 23.2 1.0 1.0 2.5
fix zwalls all wall/colloid zlo 0.0 1.0 1.0 0.858 zhi 40.0 1.0 1.0 0.858
```

16.255.3 Description

Bound the simulation domain on one or more of its faces with a flat wall that interacts with the atoms in the group by generating a force on the atom in a direction perpendicular to the wall. The energy of wall-particle interactions depends on the style.

For style *wall/lj93*, the energy E is given by the 9/3 potential:

$$E = \epsilon \left[\frac{2}{15} \left(\frac{\sigma}{r}\right)^9 - \left(\frac{\sigma}{r}\right)^3 \right] \qquad r < r_c$$

For style *wall/lj126*, the energy E is given by the 12/6 potential:

$$E = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right] \qquad r < r_c$$

For style *wall/lj1043*, the energy E is given by the 10/4/3 potential:

$$E = 2\pi\epsilon \left[\frac{2}{5} \left(\frac{\sigma}{r}\right)^{10} - \left(\frac{\sigma}{r}\right)^4 - \frac{\sqrt(2)\sigma^3}{3\left(r + \left(0.61/\sqrt(2)\right)\sigma\right)^3} \right] \qquad r < r_c$$

For style *wall/colloid*, the energy E is given by an integrated form of the *pair_style colloid* potential:

$$\begin{aligned} E =& \epsilon \left[\frac{\sigma^6}{7560} \left(\frac{6R - D}{D^7} + \frac{D + 8R}{(D + 2R)^7} \right) \right. \\ & \left. -\frac{1}{6} \left(\frac{2R(D + R) + D(D + 2R)\left[\ln D - \ln(D + 2R)\right]}{D(D + 2R)} \right) \right] \qquad r < r_c \end{aligned}$$

For style *wall/harmonic*, the energy E is given by a harmonic spring potential:

$$E = \epsilon \quad (r - r_c)^2 \qquad r < r_c$$

For style *wall/morse*, the energy E is given by a Morse potential:

$$E = D_0 \left[e^{-2\alpha(r - r_0)} - 2e^{-\alpha(r - r_0)} \right] \qquad r < r_c$$

In all cases, *r* is the distance from the particle to the wall at position *coord*, and r_c is the *cutoff* distance at which the particle and wall no longer interact. The energy of the wall potential is shifted so that the wall-particle interaction energy is 0.0 at the cutoff distance.

Up to 6 walls or faces can be specified in a single command: *xlo*, *xhi*, *ylo*, *yhi*, *zlo*, *zhi*. A *lo* face interacts with particles near the lower side of the simulation box in that dimension. A *hi* face interacts with particles near the upper side of the simulation box in that dimension.

The position of each wall can be specified in one of 3 ways: as the EDGE of the simulation box, as a constant value, or as a variable. If EDGE is used, then the corresponding boundary of the current simulation box is used. If a numeric constant is specified then the wall is placed at that position in the appropriate dimension (x, y, or z). In both the EDGE and constant cases, the wall will never move. If the wall position is a variable, it should be specified as v_name, where name is an *equal-style variable* name. In this case the variable is evaluated each timestep and the result becomes the current position of the reflecting wall. Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent wall position. See examples below.

For the *wall/lj93* and *wall/lj126* and *wall/lj1043* styles, ϵ and σ are the usual Lennard-Jones parameters, which determine the strength and size of the particle as it interacts with the wall. Epsilon has energy units. Note that this ϵ and σ may be different than any ϵ or σ values defined for a pair style that computes particle-particle interactions.

The *wall/lj93* interaction is derived by integrating over a 3d half-lattice of Lennard-Jones 12/6 particles. The *wall/lj126* interaction is effectively a harder, more repulsive wall interaction. The *wall/lj1043* interaction is yet a different form of wall interaction, described in Magda et al in *(Magda)*.

For the *wall/colloid* style, *R* is the radius of the colloid particle, *D* is the distance from the surface of the colloid particle to the wall (r-R), and σ is the size of a constituent LJ particle inside the colloid particle and wall. Note that the cutoff distance Rc in this case is the distance from the colloid particle center to the wall. The prefactor ϵ can be thought of as an effective Hamaker constant with energy units for the strength of the colloid-wall interaction. More specifically, the ϵ pre-factor is $4\pi^2\rho_{wall}\rho_{colloid}\epsilon\sigma^6$, where ϵ and σ are the LJ parameters for the constituent LJ particles. ρ_{wall} and $\rho_{colloid}$ are the number density of the constituent particles, in the wall and colloid respectively, in units of 1/volume.

The *wall/colloid* interaction is derived by integrating over constituent LJ particles of size σ within the colloid particle and a 3d half-lattice of Lennard-Jones 12/6 particles of size σ in the wall. As mentioned in the preceding paragraph, the density of particles in the wall and colloid can be different, as specified by the ϵ pre-factor.

For the *wall/harmonic* style, ϵ is effectively the spring constant K, and has units (energy/distance^2). The input parameter σ is ignored. The minimum energy position of the harmonic spring is at the *cutoff*. This is a repulsive-only spring since the interaction is truncated at the *cutoff*

For the *wall/morse* style, the three parameters are in this order: D_0 the depth of the potential, α the width parameter, and r_0 the location of the minimum. D_0 has energy units, α inverse distance units, and r_0 distance units.

For any wall, the ϵ and/or σ and/or α parameter can be specified as an *equal-style variable*, in which case it should be specified as v_name, where name is the variable name. As with a variable wall position, the variable is evaluated each timestep and the result becomes the current epsilon or sigma of the wall. Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent wall interaction.

Note: For all of the styles, you must insure that r is always > 0 for all particles in the group, or LAMMPS will generate an error. This means you cannot start your simulation with particles at the wall position *coord* (r = 0) or with particles on the wrong side of the wall (r < 0). For the *wall/lj93* and *wall/lj126* styles, the energy of the wall/particle interaction (and hence the force on the particle) blows up as r -> 0. The *wall/colloid* style is even more restrictive, since the energy blows up as D = r-R -> 0. This means the finite-size particles of radius R must be a distance larger than R from the wall position *coord*. The *harmonic* style is a softer potential and does not blow up as r -> 0, but you must use a large enough ϵ that particles always reamin on the correct side of the wall (r > 0).

The *units* keyword determines the meaning of the distance units used to define a wall position, but only when a numeric constant or variable is used. It is not relevant when EDGE is used to specify a face position. In the variable case, the variable is assumed to produce a value compatible with the *units* setting you specify.

A *box* value selects standard distance units as defined by the *units* command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacings.

The *fld* keyword can be used with a *yes* setting to invoke the wall constraint before pairwise interactions are computed. This allows an implicit FLD model using *pair_style lubricateU* to include the wall force in its calculations. If the setting is *no*, wall forces are imposed after pairwise interactions, in the usual manner.

The *pbc* keyword can be used with a *yes* setting to allow walls to be specified in a periodic dimension. See the *boundary* command for options on simulation box boundaries. The default for *pbc* is *no*, which means the system must be non-periodic when using a wall. But you may wish to use a periodic box. E.g. to allow some particles to interact with the wall via the fix group-ID, and others to pass through it and wrap around a periodic box. In this case you should insure that the wall if sufficiently far enough away from the box boundary. If you do not, then particles may interact with both the wall and with periodic images on the other side of the box, which is probably not what you want.

Here are examples of variable definitions that move the wall position in a time-dependent fashion using equal-style *variables*. The wall interaction parameters (epsilon, sigma) could be varied with additional variable definitions.

```
variable ramp equal ramp(0,10)
fix 1 all wall xlo v_ramp 1.0 1.0 2.5

variable linear equal vdisplace(0,20)
fix 1 all wall xlo v_linear 1.0 1.0 2.5

variable wiggle equal swiggle(0.0,5.0,3.0)
fix 1 all wall xlo v_wiggle 1.0 1.0 2.5

variable wiggle equal cwiggle(0.0,5.0,3.0)
fix 1 all wall xlo v_wiggle 1.0 1.0 2.5
```

The ramp(lo,hi) function adjusts the wall position linearly from lo to hi over the course of a run. The vdisplace(c0,velocity) function does something similar using the equation position = c0 + velocity*delta, where delta is the elapsed time.

The swiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation, where omega = 2 PI / period:

```
position = c0 + A sin(omega*delta)
```

The cwiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation, which will have an initial wall velocity of 0.0, and thus may impose a gentler perturbation on the particles:

```
position = c0 + A (1 - cos(omega*delta))
```

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify* *energy* option is supported by this fix to add the energy of interaction between atoms and each wall to the system's potential energy as part of *thermodynamic output*.

The *fix_modify* *virial* option is supported by this fix to add the contribution due to the interaction between atoms and each wall to the system's virial as part of *thermodynamic output*. The default is *virial no*

The *fix_modify* *respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix is adding its forces. Default is the outermost level.

This fix computes a global scalar energy and a global vector of forces, which can be accessed by various *output commands*. Note that the scalar energy is the sum of interactions with all defined walls. If you want the energy on a per-wall basis, you need to use multiple fix wall commands. The length of the vector is equal to the number of walls defined by the fix. Each vector value is the normal force on a specific wall. Note that an outward force on a wall will be a negative value for *lo* walls and a positive value for *hi* walls. The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command.

Note: If you want the atom/wall interaction energy to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the *fix_modify* *energy* option for this fix.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages*

doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

16.255.4 Restrictions

none

16.255.5 Related commands

fix wall/reflect, *fix wall/gran*, *fix wall/region*

16.255.6 Default

The option defaults units = lattice, fld = no, and pbc = no.

(Magda) Magda, Tirrell, Davis, J Chem Phys, 83, 1888-1901 (1985); erratum in JCP 84, 2901 (1986).

16.256 fix wall/body/polygon command

16.256.1 Syntax

```
fix ID group-ID wall/body/polygon k_n c_n c_t wallstyle args keyword values ...
```

- ID, group-ID are documented in *fix* command
- wall/body/polygon = style name of this fix command
- k_n = normal repulsion strength (force/distance or pressure units)
- c_n = normal damping coefficient (force/distance or pressure units)
- c_t = tangential damping coefficient (force/distance or pressure units)
- wallstyle = *xplane* or *yplane* or *zplane* or *zcylinder*
- args = list of arguments for a particular style

  ```
  xplane or yplane args = lo hi
    lo,hi = position of lower and upper plane (distance units), either can␣
  ↪be NULL)
  zcylinder args = radius
    radius = cylinder radius (distance units)
  ```

- zero or more keyword/value pairs may be appended to args

- keyword = *wiggle*

```
wiggle values = dim amplitude period
  dim = x or y or z
  amplitude = size of oscillation (distance units)
  period = time of oscillation (time units)
```

16.256.2 Examples

fix 1 all wall/body/polygon 1000.0 20.0 5.0 xplane -10.0 10.0

16.256.3 Description

This fix is for use with 2d models of body particles of style *rounded/polygon*. It bounds the simulation domain with wall(s). All particles in the group interact with the wall when they are close enough to touch it. The nature of the interaction between the wall and the polygon particles is the same as that between the polygon particles themselves, which is similar to a Hookean potential. See the *Howto body* doc page for more details on using body particles.

The parameters *k_n*, *c_n*, *c_t* have the same meaning and units as those specified with the *pair_style body/rounded/polygon* command.

The *wallstyle* can be planar or cylindrical. The 2 planar options specify a pair of walls in a dimension. Wall positions are given by *lo* and *hi*. Either of the values can be specified as NULL if a single wall is desired. For a *zcylinder* wallstyle, the cylinder's axis is at x = y = 0.0, and the radius of the cylinder is specified.

Optionally, the wall can be moving, if the *wiggle* keyword is appended.

For the *wiggle* keyword, the wall oscillates sinusoidally, similar to the oscillations of particles which can be specified by the *fix move* command. This is useful in packing simulations of particles. The arguments to the *wiggle* keyword specify a dimension for the motion, as well as it's *amplitude* and *period*. Note that if the dimension is in the plane of the wall, this is effectively a shearing motion. If the dimension is perpendicular to the wall, it is more of a shaking motion. A *zcylinder* wall can only be wiggled in the z dimension.

Each timestep, the position of a wiggled wall in the appropriate *dim* is set according to this equation:

```
position = coord + A - A cos (omega * delta)
```

where *coord* is the specified initial position of the wall, *A* is the *amplitude*, *omega* is 2 PI / *period*, and *delta* is the time elapsed since the fix was specified. The velocity of the wall is set to the derivative of this expression.

Restart, fix_modify, output, run start/stop, minimize info:

None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.256.4 Restrictions

This fix is part of the BODY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Any dimension (xy) that has a wall must be non-periodic.

16.256.5 Related commands

atom_style body, *pair_style body/rounded/polygon*

Default: none

16.257 fix wall/body/polyhedron command

16.257.1 Syntax

```
fix ID group-ID wall/body/polyhedron k_n c_n c_t wallstyle args keyword values ...
```

- ID, group-ID are documented in *fix* command
- wall/body/polyhedron = style name of this fix command
- k_n = normal repulsion strength (force/distance units or pressure units - see discussion below)
- c_n = normal damping coefficient (force/distance units or pressure units - see discussion below)
- c_t = tangential damping coefficient (force/distance units or pressure units - see discussion below)
- wallstyle = *xplane* or *yplane* or *zplane* or *zcylinder*
- args = list of arguments for a particular style

```
xplane or yplane args = lo hi
  lo,hi = position of lower and upper plane (distance units), either can␣
↪be NULL)
zcylinder args = radius
  radius = cylinder radius (distance units)
```

- zero or more keyword/value pairs may be appended to args
- keyword = *wiggle*

```
wiggle values = dim amplitude period
  dim = x or y or z
  amplitude = size of oscillation (distance units)
  period = time of oscillation (time units)
```

16.257.2 Examples

fix 1 all wall/body/polyhedron 1000.0 20.0 5.0 xplane -10.0 10.0

16.257.3 Description

This fix is for use with 3d models of body particles of style *rounded/polyhedron*. It bounds the simulation domain with wall(s). All particles in the group interact with the wall when they are close enough to touch it. The nature of the interaction between the wall and the polygon particles is the same as that between the polygon particles themselves, which is similar to a Hookean potential. See the *Howto body* doc page for more details on using body particles.

The parameters *k_n*, *c_n*, *c_t* have the same meaning and units as those specified with the *pair_style body/rounded/polyhedron* command.

The *wallstyle* can be planar or cylindrical. The 3 planar options specify a pair of walls in a dimension. Wall positions are given by *lo* and *hi*. Either of the values can be specified as NULL if a single wall is desired. For a *zcylinder* wallstyle, the cylinder's axis is at x = y = 0.0, and the radius of the cylinder is specified.

Optionally, the wall can be moving, if the *wiggle* keyword is appended.

For the *wiggle* keyword, the wall oscillates sinusoidally, similar to the oscillations of particles which can be specified by the *fix move* command. This is useful in packing simulations of particles. The arguments to the *wiggle* keyword specify a dimension for the motion, as well as it's *amplitude* and *period*. Note that if the dimension is in the plane of the wall, this is effectively a shearing motion. If the dimension is perpendicular to the wall, it is more of a shaking motion. A *zcylinder* wall can only be wiggled in the z dimension.

Each timestep, the position of a wiggled wall in the appropriate *dim* is set according to this equation:

```
position = coord + A - A cos (omega * delta)
```

where *coord* is the specified initial position of the wall, *A* is the *amplitude*, *omega* is 2 PI / *period*, and *delta* is the time elapsed since the fix was specified. The velocity of the wall is set to the derivative of this expression.

Restart, fix_modify, output, run start/stop, minimize info:

None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.257.4 Restrictions

This fix is part of the BODY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Any dimension (xyz) that has a wall must be non-periodic.

16.257.5 Related commands

atom_style body, *pair_style body/rounded/polyhedron*

Default: none

16.258 fix wall/ees command

16.259 fix wall/region/ees command

16.259.1 Syntax

```
fix ID group-ID style args
```

- ID, group-ID are documented in *fix* command
- style = *wall/ees* or *wall/region/ees*

```
args for style wall/ees: one or more face parameters groups may be␣
↪appended
face = xlo or xhi or ylo or yhi or zlo or zhi
parameters = coord epsilon sigma cutoff
  coord = position of wall = EDGE or constant or variable
```

```
      EDGE = current lo or hi edge of simulation box
      constant = number like 0.0 or -30.0 (distance units)
      variable = equal-style variable like v_x or v_wiggle
    epsilon = strength factor for wall-particle interaction (energy or␣
↪energy/distance^2 units)
      epsilon can be a variable (see below)
    sigma = size factor for wall-particle interaction (distance units)
      sigma can be a variable (see below)
    cutoff = distance from wall at which wall-particle interaction is cut␣
↪off (distance units)
  args for style wall/region/ees: region-ID epsilon sigma cutoff
    region-ID = region whose boundary will act as wall
    epsilon = strength factor for wall-particle interaction (energy or␣
↪energy/distance^2 units)
    sigma = size factor for wall-particle interaction (distance units)
    cutoff = distance from wall at which wall-particle interaction is cut␣
↪off (distance units)
```

16.259.2 Examples

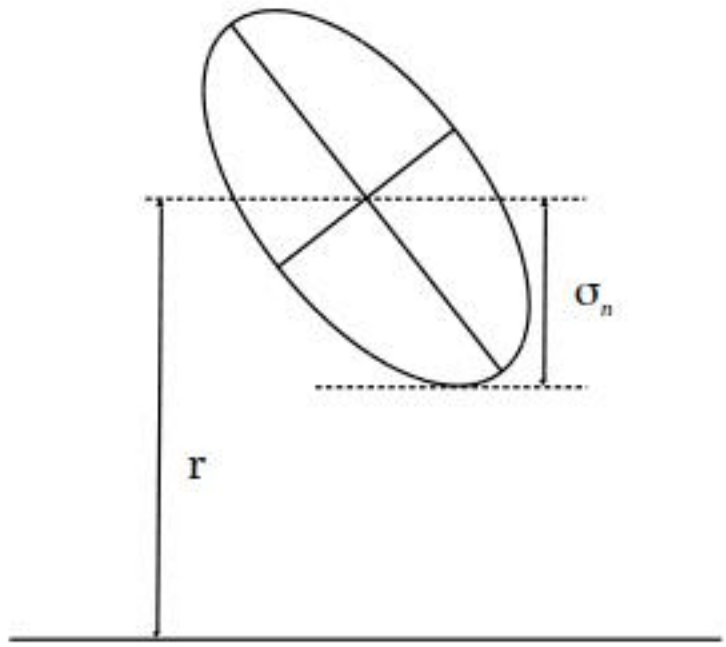
```
fix wallhi all wall/ees xlo -1.0 1.0 1.0 2.5 units box
fix wallhi all wall/ees xhi EDGE 1.0 1.0 2.5
fix wallhi all wall/ees v_wiggle 23.2 1.0 1.0 2.5
fix zwalls all wall/ees zlo 0.0 1.0 1.0 0.858 zhi 40.0 1.0 1.0 0.858

fix ees_cube all wall/region/ees myCube 1.0 1.0 2.5
```

16.259.3 Description

Fix *wall/ees* bounds the simulation domain on one or more of its faces with a flat wall that interacts with the ellipsoidal atoms in the group by generating a force on the atom in a direction perpendicular to the wall and a torque parallel with the wall. The energy of wall-particle interactions E is given by:

$$E = \epsilon \left[\frac{2\sigma_{LJ}^{12}\left(7r^5 + 14r^3\sigma_n^2 + 3r\sigma_n^4\right)}{945\left(r^2 - \sigma_n^2\right)^7} - \frac{\sigma_{LJ}^6\left(2r\sigma_n^3 + \sigma_n^2\left(r^2 - \sigma_n^2\right)\log\left[\frac{r-\sigma_n}{r+\sigma_n}\right]\right)}{12\sigma_n^5\left(r^2 - \sigma_n^2\right)} \right] \qquad \sigma_n < r < r_c$$

Introduced by Babadi and Ejtehadi in *(Babadi)*. Here, *r* is the distance from the particle to the wall at position *coord*, and Rc is the *cutoff* distance at which the particle and wall no longer interact. Also, σ_n is the distance between center of ellipsoid and the nearest point of its surface to the wall as shown below.



Details of using this command and specifications are the same as fix/wall command. You can also find an example in USER/ees/ under examples/ directory.

The prefactor ϵ can be thought of as an effective Hamaker constant with energy units for the strength of the ellipsoid-wall interaction. More specifically, the ϵ pre-factor is

$$8\pi^2 \quad \rho_{wall} \quad \rho_{ellipsoid} \quad \epsilon \quad \sigma_a \quad \sigma_b \quad \sigma_c$$

where ϵ is the LJ energy parameter for the constituent LJ particles and σ_a, σ_b, and σ_c are the radii of the ellipsoidal particles. ρ_{wall} and $\rho_{ellipsoid}$ are the number density of the constituent particles, in the wall and ellipsoid respectively, in units of 1/volume.

Note: You must insure that r is always bigger than σ_n for all particles in the group, or LAMMPS will generate an error. This means you cannot start your simulation with particles touching the wall position *coord* ($r = \sigma_n$) or with particles penetrating the wall ($0 =< r < \sigma_n$) or with particles on the wrong side of the wall ($r < 0$).

Fix *wall/region/ees* treats the surface of the geometric region defined by the *region-ID* as a bounding wall which interacts with nearby ellipsoidal particles according to the EES potential introduced above.

Other details of this command are the same as for the *fix wall/region* command. One may also find an example of using this fix in the examples/USER/misc/ees/ directory.

16.259.4 Restrictions

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This fix requires that atoms be ellipsoids as defined by the *atom_style ellipsoid* command.

16.259.5 Related commands

fix wall, *pair resquared*

16.259.6 Default

none

(Babadi) Babadi and Ejtehadi, EPL, 77 (2007) 23002.

16.260 fix wall/gran command

16.260.1 Syntax

```
fix ID group-ID wall/gran fstyle fstyle_params wallstyle args keyword values ...
```

- ID, group-ID are documented in *fix* command
- wall/gran = style name of this fix command
- fstyle = style of force interactions between particles and wall

```
possible choices: hooke, hooke/history, hertz/history, granular
```

- fstyle_params = parameters associated with force interaction style

```
For hooke, hooke/history, and hertz/history, fstyle_params are:
      Kn = elastic constant for normal particle repulsion (force/distance␣
↪units or pressure units - see discussion below)
      Kt = elastic constant for tangential contact (force/distance units␣
↪or pressure units - see discussion below)
      gamma_n = damping coefficient for collisions in normal direction (1/
↪time units or 1/time-distance units - see discussion below)
      gamma_t = damping coefficient for collisions in tangential␣
↪direction (1/time units or 1/time-distance units - see discussion below)
      xmu = static yield criterion (unitless value between 0.0 and 1.0e4)
      dampflag = 0 or 1 if tangential damping force is excluded or␣
↪included

For granular, fstyle_params are set using the same syntax as for the pair_
↪coeff command of pair_style granular
```

- wallstyle = *xplane* or *yplane* or *zplane* or *zcylinder*
- args = list of arguments for a particular style

```
xplane or yplane or zplane args = lo hi
  lo,hi = position of lower and upper plane (distance units), either can␣
↪be NULL)
zcylinder args = radius
  radius = cylinder radius (distance units)
```

- zero or more keyword/value pairs may be appended to args
- keyword = *wiggle* or *shear*

```
wiggle values = dim amplitude period
  dim = x or y or z
  amplitude = size of oscillation (distance units)
  period = time of oscillation (time units)
shear values = dim vshear
  dim = x or y or z
  vshear = magnitude of shear velocity (velocity units)
```

16.260.2 Examples

```
fix 1 all wall/gran hooke  200000.0 NULL 50.0 NULL 0.5 0 xplane -10.0 10.0
fix 1 all wall/gran hooke/history 200000.0 NULL 50.0 NULL 0.5 0 zplane 0.0 NULL
fix 2 all wall/gran hooke 100000.0 20000.0 50.0 30.0 0.5 1 zcylinder 15.0 wiggle z 3.
↪0 2.0
fix 3 all wall/gran/region granular hooke 1000.0 50.0 tangential linear_nohistory 1.0␣
↪0.4 damping velocity region myBox
fix 4 all wall/gran/region granular jkr 1e5 1500.0 0.3 10.0 tangential mindlin NULL 1.
↪0 0.5 rolling sds 500.0 200.0 0.5 twisting marshall region myCone
fix 5 all wall/gran/region granular dmt 1e5 0.2 0.3 10.0 tangential mindlin NULL 1.0␣
↪0.5 rolling sds 500.0 200.0 0.5 twisting marshall damping tsuji region myCone
```

16.260.3 Description

Bound the simulation domain of a granular system with a frictional wall. All particles in the group interact with the wall when they are close enough to touch it.

The nature of the wall/particle interactions are determined by the *fstyle* setting. It can be any of the styles defined by the *pair_style gran/** or the more general *pair_style granular* commands. Currently the options are *hooke*, *hooke/history*, or *hertz/history* for the former, and *granular* with all the possible options of the associated *pair_coeff* command for the latter. The equation for the force between the wall and particles touching it is the same as the corresponding equation on the *pair_style gran/** and *pair_style granular* doc pages, in the limit of one of the two particles going to infinite radius and mass (flat wall). Specifically, delta = radius - r = overlap of particle with wall, m_eff = mass of particle, and the effective radius of contact = RiRj/Ri+Rj is set to the radius of the particle.

The parameters *Kn*, *Kt*, *gamma_n*, *gamma_t*, *xmu* and *dampflag* have the same meaning and units as those specified with the *pair_style gran/** commands. This means a NULL can be used for either *Kt* or *gamma_t* as described on that page. If a NULL is used for *Kt*, then a default value is used where *Kt* = 2/7 *Kn*. If a NULL is used for *gamma_t*, then a default value is used where *gamma_t* = 1/2 *gamma_n*.

All the model choices for cohesion, tangential friction, rolling friction and twisting friction supported by the *pair_style granular* through its *pair_coeff* command are also supported for walls. These are discussed in greater detail on the doc page for *pair_style granular*.

Note that you can choose a different force styles and/or different values for the wall/particle coefficients than for particle/particle interactions. E.g. if you wish to model the wall as a different material.

Note: As discussed on the doc page for *pair_style gran/**, versions of LAMMPS before 9Jan09 used a different equation for Hertzian interactions. This means Hertizian wall/particle interactions have also changed. They now include a sqrt(radius) term which was not present before. Also the previous versions used Kn and Kt from the pairwise interaction and hardwired dampflag to 1, rather than letting them be specified directly. This means you can set the values of the wall/particle coefficients appropriately in the current code to reproduce the results of a previous Hertzian monodisperse calculation. For example, for the common case of a monodisperse system with particles of diameter 1, Kn, Kt, gamma_n, and gamma_s should be set sqrt(2.0) larger than they were previously.

The effective mass *m_eff* in the formulas listed on the *pair_style granular* doc page is the mass of the particle for particle/wall interactions (mass of wall is infinite). If the particle is part of a rigid body, its mass is replaced by the mass of the rigid body in those formulas. This is determined by searching for a *fix rigid* command (or its variants).

The *wallstyle* can be planar or cylindrical. The 3 planar options specify a pair of walls in a dimension. Wall positions are given by *lo* and *hi*. Either of the values can be specified as NULL if a single wall is desired. For a *zcylinder* wallstyle, the cylinder's axis is at x = y = 0.0, and the radius of the cylinder is specified.

Optionally, the wall can be moving, if the *wiggle* or *shear* keywords are appended. Both keywords cannot be used together.

For the *wiggle* keyword, the wall oscillates sinusoidally, similar to the oscillations of particles which can be specified by the *fix move* command. This is useful in packing simulations of granular particles. The arguments to the *wiggle* keyword specify a dimension for the motion, as well as it's *amplitude* and *period*. Note that if the dimension is in the plane of the wall, this is effectively a shearing motion. If the dimension is perpendicular to the wall, it is more of a shaking motion. A *zcylinder* wall can only be wiggled in the z dimension.

Each timestep, the position of a wiggled wall in the appropriate *dim* is set according to this equation:

```
position = coord + A - A cos (omega * delta)
```

where *coord* is the specified initial position of the wall, *A* is the *amplitude*, *omega* is 2 PI / *period*, and *delta* is the time elapsed since the fix was specified. The velocity of the wall is set to the derivative of this expression.

For the *shear* keyword, the wall moves continuously in the specified dimension with velocity *vshear*. The dimension must be tangential to walls with a planar *wallstyle*, e.g. in the *y* or *z* directions for an *xplane* wall. For *zcylinder* walls, a dimension of *z* means the cylinder is moving in the z-direction along it's axis. A dimension of *x* or *y* means the cylinder is spinning around the z-axis, either in the clockwise direction for *vshear* > 0 or counter-clockwise for *vshear* < 0. In this case, *vshear* is the tangential velocity of the wall at whatever *radius* has been defined.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the shear friction state of atoms interacting with the wall to *binary restart files*, so that a simulation can continue correctly if granular potentials with shear "history" effects are being used. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.260.4 Restrictions

This fix is part of the GRANULAR package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Any dimension (xyz) that has a granular wall must be non-periodic.

16.260.5 Related commands

fix move, *fix wall/gran/region*, *pair_style gran/** *pair_style granular*

Default: none

16.261 fix wall/gran/region command

16.261.1 Syntax

```
fix ID group-ID wall/gran/region fstyle fstyle_params wallstyle regionID
```

- ID, group-ID are documented in *fix* command
- wall/region = style name of this fix command
- fstyle = style of force interactions between particles and wall

```
possible choices: hooke, hooke/history, hertz/history, granular
```

- fstyle_params = parameters associated with force interaction style

```
For hooke, hooke/history, and hertz/history, fstyle_params are:
      Kn = elastic constant for normal particle repulsion (force/distance␣
↪units or pressure units - see discussion below)
      Kt = elastic constant for tangential contact (force/distance units␣
↪or pressure units - see discussion below)
      gamma_n = damping coefficient for collisions in normal direction (1/
↪time units or 1/time-distance units - see discussion below)
      gamma_t = damping coefficient for collisions in tangential␣
↪direction (1/time units or 1/time-distance units - see discussion below)
      xmu = static yield criterion (unitless value between 0.0 and 1.0e4)
      dampflag = 0 or 1 if tangential damping force is excluded or␣
↪included

For granular, fstyle_params are set using the same syntax as for the pair_
↪coeff command of pair_style granular
```

- wallstyle = region (see *fix wall/gran* for options for other kinds of walls)
- region-ID = region whose boundary will act as wall

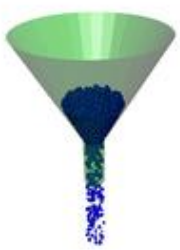
16.261.2 Examples

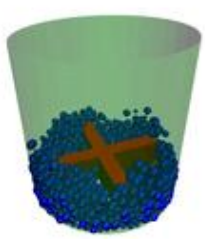
```
fix wall all wall/gran/region hooke/history 1000.0 200.0 200.0 100.0 0.5 1 region␣
↪myCone
fix 3 all wall/gran/region granular hooke 1000.0 50.0 tangential linear_nohistory 1.0␣
↪0.4 damping velocity region myBox
fix 4 all wall/gran/region granular jkr 1e5 1500.0 0.3 10.0 tangential mindlin NULL 1.
↪0 0.5 rolling sds 500.0 200.0 0.5 twisting marshall region myCone
fix 5 all wall/gran/region granular dmt 1e5 0.2 0.3 10.0 tangential mindlin NULL 1.0␣
↪0.5 rolling sds 500.0 200.0 0.5 twisting marshall damping tsuji region myCone
```

16.261.3 Description

Treat the surface of the geometric region defined by the *region-ID* as a bounding frictional wall which interacts with nearby finite-size granular particles when they are close enough to touch the wall. See the *fix wall/region* and *fix wall/gran* commands for related kinds of walls for non-granular particles and simpler wall geometries, respectively.

Here are snapshots of example models using this command. Corresponding input scripts can be found in examples/granregion. Click on the images to see a bigger picture. Movies of these simulations are here on the Movies page of the LAMMPS web site.





The distance between a particle and the region boundary is the distance to the nearest point on the region surface. The force the wall exerts on the particle is along the direction between that point and the particle center, which is the direction normal to the surface at that point. Note that if the region surface is comprised of multiple "faces", then each face can exert a force on the particle if it is close enough. E.g. for *region_style block*, a particle in the interior, near a corner of the block, could feel wall forces from 1, 2, or 3 faces of the block.

Regions are defined using the *region* command. Note that the region volume can be interior or exterior to the bounding surface, which will determine in which direction the surface interacts with particles, i.e. the direction of the surface normal. The exception to this is if one or more *open* options are specified for the region command, in which case particles interact with both the interior and exterior surfaces of regions.

Regions can either be primitive shapes (block, sphere, cylinder, etc) or combinations of primitive shapes specified via the *union* or *intersect* region styles. These latter styles can be used to construct particle containers with complex shapes.

Regions can also move dynamically via the *region* command keywords (move) and *rotate*, or change their shape by use of variables as inputs to the *region* command. If such a region is used with this fix, then the region surface will move in time in the corresponding manner.

Note: As discussed on the *region* command doc page, regions in LAMMPS do not get wrapped across periodic boundaries. It is up to you to ensure that the region location with respect to periodic or non-periodic boundaries is specified appropriately via the *region* and *boundary* commands when using a region as a wall that bounds particle motion.

Note: For primitive regions with sharp corners and/or edges (e.g. a block or cylinder), wall/particle forces are computed accurately for both interior and exterior regions. For *union* and *intersect* regions, additional sharp corners and edges may be present due to the intersection of the surfaces of 2 or more primitive volumes. These corners and edges can be of two types: concave or convex. Concave points/edges are like the corners of a cube as seen by particles in the interior of a cube. Wall/particle forces around these features are computed correctly. Convex points/edges are like the corners of a cube as seen by particles exterior to the cube, i.e. the points jut into the volume where particles are present. LAMMPS does NOT compute the location of these convex points directly, and hence wall/particle forces in the cutoff volume around these points suffer from inaccuracies. The basic problem is that the outward normal of the surface is not continuous at these points. This can cause particles to feel no force (they don't "see" the wall) when in one location, then move a distance epsilon, and suddenly feel a large force because they now "see" the wall. In a worst-case scenario, this can blow particles out of the simulation box. Thus, as a general rule you should not use the fix wall/gran/region command with *union* or *interesect* regions that have convex points or edges resulting from the union/intersection (convex points/edges in the union/intersection due to a single sub-region are still OK).

Note: Similarly, you should not define *union* or *intersert* regions for use with this command that share an overlapping common face that is part of the overall outer boundary (interior boundary is OK), even if the face is smooth. E.g. two regions of style block in a *union* region, where the two blocks overlap on one or more of their faces. This is because LAMMPS discards points that are part of multiple sub-regions when calculating wall/particle interactions, to avoid double-counting the interaction. Having two coincident faces could cause the face to become invisible to the particles. The solution is to make the two faces differ by epsilon in their position.

The nature of the wall/particle interactions are determined by the *fstyle* setting. It can be any of the styles defined by the *pair_style gran/** or the more general *pair_style granular* commands. Currently the options are *hooke*, *hooke/history*, or *hertz/history* for the former, and *granular* with all the possible options of the associated *pair_coeff* command for the latter. The equation for the force between the wall and particles touching it is the same as the corresponding equation on the *pair_style gran/** and *pair_style granular* doc pages, but the effective radius is calculated using the radius of the particle and the radius of curvature of the wall at the contact point.

Specifically, delta = radius - r = overlap of particle with wall, m_eff = mass of particle, and RiRj/Ri+Rj is the effective radius, with Rj replaced by the radius of curvature of the wall at the contact point. The radius of curvature can be negative for a concave wall section, e.g. the interior of cylinder. For a flat wall, delta = radius - r = overlap of particle with wall, m_eff = mass of particle, and the effective radius of contact is just the radius of the particle.

The parameters *Kn*, *Kt*, *gamma_n*, *gamma_t*, *xmu* and *dampflag* have the same meaning and units as those specified

with the *pair_style gran/** commands. This means a NULL can be used for either *Kt* or *gamma_t* as described on that page. If a NULL is used for *Kt*, then a default value is used where *Kt* = 2/7 *Kn*. If a NULL is used for *gamma_t*, then a default value is used where *gamma_t* = 1/2 *gamma_n*.

All the model choices for cohesion, tangential friction, rolling friction and twisting friction supported by the *pair_style granular* through its *pair_coeff* command are also supported for walls. These are discussed in greater detail on the doc page for *pair_style granular*.

Note that you can choose a different force styles and/or different values for the 6 wall/particle coefficients than for particle/particle interactions. E.g. if you wish to model the wall as a different material.

Restart, fix_modify, output, run start/stop, minimize info:

Similar to *fix wall/gran* command, this fix writes the shear friction state of atoms interacting with the wall to *binary restart files*, so that a simulation can continue correctly if granular potentials with shear "history" effects are being used. This fix also includes info about a moving region in the restart file. See the *read_restart* command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

Note: Information about region definitions is NOT included in restart files, as discussed on the *read_restart* doc page. So you must re-define your region and if it is a moving region, define its motion attributes in a way that is consistent with the simulation that wrote the restart file. In particular, if you want to change the region motion attributes (e.g. its velocity), then you should ensure the position/orientation of the region at the initial restart timestep is the same as it was on the timestep the restart file was written. If this is not possible, you may need to ignore info in the restart file by defining a new fix wall/gran/region command in your restart script, e.g. with a different fix ID. Or if you want to keep the shear history info but discard the region motion information, you can use the same fix ID for fix wall/gran/region, but assign it a region with a different region ID.

None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.261.4 Restrictions

This fix is part of the GRANULAR package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.261.5 Related commands

fix_move, *fix wall/gran*, *fix wall/region*, *pair_style granular*, *region*

Default: none

16.262 fix wall/piston command

16.262.1 Syntax

```
fix ID group-ID wall/piston face ... keyword value ...
```

- ID, group-ID are documented in *fix* command
- wall/piston = style name of this fix command

- face = *zlo*
- zero or more keyword/value pairs may be appended
- keyword = *pos* or *vel* or *ramp* or *units*

```
pos args = z
  z = z coordinate at which the piston begins (distance units)
vel args = vz
  vz = final velocity of the piston (velocity units)
ramp = use a linear velocity ramp from 0 to vz
temp args = target damp seed extent
  target = target velocity for region immediately ahead of the piston
  damp = damping parameter (time units)
  seed = random number seed for langevin kicks
  extent = extent of thermostatted region (distance units)
units value = lattice or box
  lattice = the wall position is defined in lattice units
  box = the wall position is defined in simulation box units
```

16.262.2 Examples

```
fix xwalls all wall/piston zlo
fix walls all wall/piston zlo pos 1.0 vel 10.0 units box
fix top all wall/piston zlo vel 10.0 ramp
```

16.262.3 Description

Bound the simulation with a moving wall which reflect particles in the specified group and drive the system with an effective infinite-mass piston capable of driving shock waves.

A momentum mirror technique is used, which means that if an atom (or the wall) moves such that an atom is outside the wall on a timestep by a distance delta (e.g. due to *fix nve*), then it is put back inside the face by the same delta, and the velocity relative to the moving wall is flipped in z. For instance, a stationary particle hit with a piston wall with velocity vz, will end the timestep with a velocity of 2*vz.

Currently the *face* keyword can only be *zlo*. This creates a piston moving in the positive z direction. Particles with z coordinate less than the wall position are reflected to a z coordinate greater than the wall position. If the piston velocity is vpz and the particle velocity before reflection is vzi, the particle velocity after reflection is -vzi + 2*vpz.

The initial position of the wall can be specified by the *pos* keyword.

The final velocity of the wall can be specified by the *vel* keyword

The *ramp* keyword will cause the wall/piston to adjust the velocity linearly from zero velocity to *vel* over the course of the run. If the *ramp* keyword is omitted then the wall/piston moves at a constant velocity defined by *vel*.

The *temp* keyword will cause the region immediately in front of the wall/piston to be thermostatted with a Langevin thermostat. This region moves with the piston. The damping and kicking are measured in the reference frame of the piston. So, a temperature of zero would mean all particles were moving at exactly the speed of the wall/piston.

The *units* keyword determines the meaning of the distance units used to define a wall position, but only when a numeric constant is used.

A *box* value selects standard distance units as defined by the *units* command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacings.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.262.4 Restrictions

This fix style is part of the SHOCK package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

The face that has the wall/piston must be boundary type 's' (shrink-wrapped). The opposing face can be any boundary type other than periodic.

A wall/piston should not be used with rigid bodies such as those defined by a "fix rigid" command. This is because the wall/piston displaces atoms directly rather than exerting a force on them.

16.262.5 Related commands

fix wall/reflect command, *fix append/atoms* command

16.262.6 Default

The keyword defaults are pos = 0, vel = 0, units = lattice.

16.263 fix wall/reflect command

16.264 fix wall/reflect/kk command

16.264.1 Syntax

```
fix ID group-ID wall/reflect face arg ... keyword value ...
```

- ID, group-ID are documented in *fix* command
- wall/reflect = style name of this fix command
- one or more face/arg pairs may be appended
- face = *xlo* or *xhi* or *ylo* or *yhi* or *zlo* or *zhi*

```
arg = EDGE or constant or variable
  EDGE = current lo edge of simulation box
  constant = number like 0.0 or 30.0 (distance units)
  variable = equal-style variable like v_x or v_wiggle
```

- zero or more keyword/value pairs may be appended
- keyword = *units*

```
units value = lattice or box
  lattice = the wall position is defined in lattice units
  box = the wall position is defined in simulation box units
```

16.264.2 Examples

```
fix xwalls all wall/reflect xlo EDGE xhi EDGE
fix walls all wall/reflect xlo 0.0 ylo 10.0 units box
fix top all wall/reflect zhi v_pressdown
```

16.264.3 Description

Bound the simulation with one or more walls which reflect particles in the specified group when they attempt to move through them.

Reflection means that if an atom moves outside the wall on a timestep by a distance delta (e.g. due to *fix nve*), then it is put back inside the face by the same delta, and the sign of the corresponding component of its velocity is flipped.

When used in conjunction with *fix nve* and *run_style verlet*, the resultant time-integration algorithm is equivalent to the primitive splitting algorithm (PSA) described by *Bond*. Because each reflection event divides the corresponding timestep asymmetrically, energy conservation is only satisfied to O(dt), rather than to O(dt^2) as it would be for velocity-Verlet integration without reflective walls.

Up to 6 walls or faces can be specified in a single command: *xlo*, *xhi*, *ylo*, *yhi*, *zlo*, *zhi*. A *lo* face reflects particles that move to a coordinate less than the wall position, back in the *hi* direction. A *hi* face reflects particles that move to a coordinate higher than the wall position, back in the *lo* direction.

The position of each wall can be specified in one of 3 ways: as the EDGE of the simulation box, as a constant value, or as a variable. If EDGE is used, then the corresponding boundary of the current simulation box is used. If a numeric constant is specified then the wall is placed at that position in the appropriate dimension (x, y, or z). In both the EDGE and constant cases, the wall will never move. If the wall position is a variable, it should be specified as v_name, where name is an *equal-style variable* name. In this case the variable is evaluated each timestep and the result becomes the current position of the reflecting wall. Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent wall position.

The *units* keyword determines the meaning of the distance units used to define a wall position, but only when a numeric constant or variable is used. It is not relevant when EDGE is used to specify a face position. In the variable case, the variable is assumed to produce a value compatible with the *units* setting you specify.

A *box* value selects standard distance units as defined by the *units* command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacings.

Here are examples of variable definitions that move the wall position in a time-dependent fashion using equal-style *variables*.

```
variable ramp equal ramp(0,10)
fix 1 all wall/reflect xlo v_ramp

variable linear equal vdisplace(0,20)
fix 1 all wall/reflect xlo v_linear
```

(continues on next page)

(continued from previous page)

```
variable wiggle equal swiggle(0.0,5.0,3.0)
fix 1 all wall/reflect xlo v_wiggle

variable wiggle equal cwiggle(0.0,5.0,3.0)
fix 1 all wall/reflect xlo v_wiggle
```

The ramp(lo,hi) function adjusts the wall position linearly from lo to hi over the course of a run. The vdisplace(c0,velocity) function does something similar using the equation position = c0 + velocity*delta, where delta is the elapsed time.

The swiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation, where omega = 2 PI / period:

```
position = c0 + A sin(omega*delta)
```

The cwiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation, which will have an initial wall velocity of 0.0, and thus may impose a gentler perturbation on the particles:

```
position = c0 + A (1 - cos(omega*delta))
```

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various *output commands*. No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.264.4 Restrictions

Any dimension (xyz) that has a reflecting wall must be non-periodic.

A reflecting wall should not be used with rigid bodies such as those defined by a "fix rigid" command. This is because the wall/reflect displaces atoms directly rather than exerts a force on them. For rigid bodies, use a soft wall instead, such as *fix wall/lj93*. LAMMPS will flag the use of a rigid fix with fix wall/reflect with a warning, but will not generate an error.

16.264.5 Related commands

fix wall/lj93, *fix oneway*

Default:

The default for the units keyword is lattice.

(Bond) Bond and Leimkuhler, SIAM J Sci Comput, 30, p 134 (2007).

16.265 fix wall/reflect/stochastic command

16.265.1 Syntax

```
fix ID group-ID wall/reflect/stochastic rstyle seed face args ... keyword value ...
```

- ID, group-ID are documented in *fix* command
- wall/reflect/stochastic = style name of this fix command
- rstyle = diffusive or maxwell or ccl
- seed = random seed for stochasticity (positive integer)
- one or more face/args pairs may be appended
- face = *xlo* or *xhi* or *ylo* or *yhi* or *zlo* or *zhi*

```
args = pos temp velx vely velz accomx accomy accomz
  pos = EDGE or constant
    EDGE = current lo or hi edge of simulation box
    constant = number like 0.0 or 30.0 (distance units)
  temp = wall temperature (temperature units)
  velx,vely,velz = wall velocity in x,y,z directions (velocity units)
  accomx,accomy,accomz = accommodation coeffs in x,y,z directions (unitless)
    not specified for rstyle = diffusive
    single accom coeff specified for rstyle maxwell
    all 3 coeffs specified for rstyle cll
```

- zero or more keyword/value pairs may be appended
- keyword = *units*

```
units value = lattice or box
  lattice = the wall position is defined in lattice units
  box = the wall position is defined in simulation box units
```

16.265.2 Examples

```
fix zwalls all wall/reflect/stochastic diffusive 23424 zlo EDGE 300 0.1 0.1 0 zhi␣
↪EDGE 200 0.1 0.1 0
fix ywalls all wall/reflect/stochastic maxwell 345533 ylo 5.0 300 0.1 0.0 0.0 0.8 yhi␣
↪10.0 300 0.1 0.0 0.0 0.8
fix xwalls all wall/reflect/stochastic cercignanilampis 2308 xlo 0.0 300 0.0 0.1 0.9␣
↪0.8 0.7 xhi EDGE 300 0.0 0.1 0 0.9 0.8 0.7 units box
```

16.265.3 Description

Bound the simulation with one or more walls which reflect particles in the specified group when they attempt to move through them.

Reflection means that if an atom moves outside the wall on a timestep (e.g. due to the *fix nve* command), then it is put back inside the wall with a changed velocity.

This fix models treats the wall as a moving solid boundary with a finite temperature, which can exchange energy with particles that collide with it. This is different than the simpler *fix wall/reflect* command which models mirror reflection. For this fix, the post collision velocity of each particle is treated stochastically. The randomness can come from many sources: thermal motion of the wall atoms, surface roughness, etc. Three stochastic reflection models are currently implemented.

For rstyle *diffusive*, particles are reflected diffusively. Their velocity distribution corresponds to an equilibrium distribution of particles at the wall temperature. No accommodation coefficients are specified.

For rstyle *maxwell*, particle reflection is Maxwellian which means partially diffusive and partially specular (*Maxwell*). A single accommodation coeff is specified which must be between 0.0 and 1.0 inclusive. It determines the fraction of the collision which is diffusive versus specular. An accommodation coefficient of 1.0 is fully diffusive; a coefficient of 0.0 is fully specular.

For rstyle *cll*, particle collisions are computed by the Cercignani/Lampis model. See *CL* and *To* for details. Three accommodations coefficient are specified. Each must be between 0.0 and 1.0 inclusive. Two are velocity accommodation coefficients; one is a normal kinetic energy accommodation. The normal coeff is the one corresponding to the normal of the wall itself. For example if the wall is *ylo* or *yhi*, *accomx* and *accomz* are the tangential velocity accommodation coefficients, and *accomy* is the normal kinetic energy accommodation coefficient.

The optional *units* keyword determines the distance units used to define a wall position. A *box* value selects standard distance units as defined by the *units* command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacings.

16.265.4 Restrictions

This fix has the same limitations as the *fix wall/reflect* command. Any dimension (xyz) that has a wall must be non-periodic. It should not be used with rigid bodies such as those defined by the *fix rigid* command. The wall velocity must lie on the same plane as the wall itself.

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

16.265.5 Related commands

fix wall/reflect

16.265.6 Default

The default for the units keyword is lattice.

(Maxwell) J.C. Maxwell, Philos. Tans. Royal Soc. London, 157: 49-88 (1867).

(Cercignani) C. Cercignani and M. Lampis. Trans. Theory Stat. Phys. 1, 2, 101 (1971).

(To) Q.D. To, V.H. Vu, G. Lauriat, and C. Leonard. J. Math. Phys. 56, 103101 (2015).

16.266 fix wall/region command

16.266.1 Syntax

```
fix ID group-ID wall/region region-ID style args ... cutoff
```

- ID, group-ID are documented in *fix* command
- wall/region = style name of this fix command
- region-ID = region whose boundary will act as wall
- style = *lj93* or *lj126* or *lj1043* or *colloid* or *harmonic* or *morse*
- args for styles *lj93* or *lj126* or *lj1043* or *colloid* or *harmonic* =

  ```
  epsilon = strength factor for wall-particle interaction (energy or energy/
  ↪distance^2 units)
  sigma = size factor for wall-particle interaction (distance units)
  ```

- args for style *morse* =

  ```
  D_0 = depth of the potential (energy units)
  alpha = width parameter (1/distance units)
  r_0 = distance of the potential minimum from wall position (distance units)
  ```

- cutoff = distance from wall at which wall-particle interaction is cut off (distance units)

16.266.2 Examples

```
fix wall all wall/region mySphere lj93 1.0 1.0 2.5
fix wall all wall/region mySphere harmonic 1.0 0.0 2.5
fix wall all wall/region box_top morse 1.0 1.0 1.5 3.0
```

16.266.3 Description

Treat the surface of the geometric region defined by the *region-ID* as a bounding wall which interacts with nearby particles according to the specified style.

The distance between a particle and the surface is the distance to the nearest point on the surface and the force the wall exerts on the particle is along the direction between that point and the particle, which is the direction normal to the surface at that point. Note that if the region surface is comprised of multiple "faces", then each face can exert a force on the particle if it is close enough. E.g. for *region_style block*, a particle in the interior, near a corner of the block, could feel wall forces from 1, 2, or 3 faces of the block.

Regions are defined using the *region* command. Note that the region volume can be interior or exterior to the bounding surface, which will determine in which direction the surface interacts with particles, i.e. the direction of the surface normal. The surface of the region only exerts forces on particles "inside" the region; if a particle is "outside" the region it will generate an error, because it has moved through the wall.

Regions can either be primitive shapes (block, sphere, cylinder, etc) or combinations of primitive shapes specified via the *union* or *intersect* region styles. These latter styles can be used to construct particle containers with complex shapes. Regions can also change over time via the *region* command keywords (move) and *rotate*. If such a region is used with this fix, then the of region surface will move over time in the corresponding manner.

Note: As discussed on the *region* command doc page, regions in LAMMPS do not get wrapped across periodic boundaries. It is up to you to insure that periodic or non-periodic boundaries are specified appropriately via the *boundary* command when using a region as a wall that bounds particle motion. This also means that if you embed a region in your simulation box and want it to repulse particles from its surface (using the "side out" option in the *region* command), that its repulsive force will not be felt across a periodic boundary.

Note: For primitive regions with sharp corners and/or edges (e.g. a block or cylinder), wall/particle forces are computed accurately for both interior and exterior regions. For *union* and *intersect* regions, additional sharp corners and edges may be present due to the intersection of the surfaces of 2 or more primitive volumes. These corners and edges can be of two types: concave or convex. Concave points/edges are like the corners of a cube as seen by particles in the interior of a cube. Wall/particle forces around these features are computed correctly. Convex points/edges are like the corners of a cube as seen by particles exterior to the cube, i.e. the points jut into the volume where particles are present. LAMMPS does NOT compute the location of these convex points directly, and hence wall/particle forces in the cutoff volume around these points suffer from inaccuracies. The basic problem is that the outward normal of the surface is not continuous at these points. This can cause particles to feel no force (they don't "see" the wall) when in one location, then move a distance epsilon, and suddenly feel a large force because they now "see" the wall. In a worst-case scenario, this can blow particles out of the simulation box. Thus, as a general rule you should not use the fix wall/gran/region command with *union* or *interesect* regions that have convex points or edges resulting from the union/intersection (convex points/edges in the union/intersection due to a single sub-region are still OK).

Note: Similarly, you should not define *union* or *intersert* regions for use with this command that share an overlapping common face that is part of the overall outer boundary (interior boundary is OK), even if the face is smooth. E.g. two regions of style block in a *union* region, where the two blocks overlap on one or more of their faces. This is because LAMMPS discards points that are part of multiple sub-regions when calculating wall/particle interactions, to avoid double-counting the interaction. Having two coincident faces could cause the face to become invisible to the particles. The solution is to make the two faces differ by epsilon in their position.

The energy of wall-particle interactions depends on the specified style.

For style *lj93*, the energy E is given by the 9/3 potential:

$$E = \epsilon \left[\frac{2}{15} \left(\frac{\sigma}{r}\right)^9 - \left(\frac{\sigma}{r}\right)^3 \right] \qquad r < r_c$$

For style *lj126*, the energy E is given by the 12/6 potential:

$$E = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right] \qquad r < r_c$$

For style *wall/lj1043*, the energy E is given by the 10/4/3 potential:

$$E = 2\pi\epsilon \left[\frac{2}{5} \left(\frac{\sigma}{r}\right)^{10} - \left(\frac{\sigma}{r}\right)^4 - \frac{\sqrt(2)\sigma^3}{3\left(r + \left(0.61/\sqrt(2)\right)\sigma\right)^3} \right] \qquad r < r_c$$

For style *colloid*, the energy E is given by an integrated form of the *pair_style colloid* potential:

$$\begin{aligned} E =& \epsilon \left[\frac{\sigma^6}{7560} \left(\frac{6R - D}{D^7} + \frac{D + 8R}{(D + 2R)^7} \right) \right. \\ & \left. -\frac{1}{6} \left(\frac{2R(D + R) + D(D + 2R)\left[\ln D - \ln(D + 2R)\right]}{D(D + 2R)} \right) \right] \qquad r < r_c \end{aligned}$$

For style *wall/harmonic*, the energy E is given by a harmonic spring potential (the distance parameter is ignored):

$$E = \epsilon \quad (r - r_c)^2 \qquad r < r_c$$

For style *wall/morse*, the energy E is given by the Morse potential:

$$E = D_0 \left[e^{-2\alpha(r - r_0)} - 2e^{-\alpha(r - r_0)} \right] \qquad r < r_c$$

Unlike other styles, this requires three parameters (D_0, α, and r_0 in this order) instead of two like for the other wall styles.

In all cases, *r* is the distance from the particle to the region surface, and Rc is the *cutoff* distance at which the particle and surface no longer interact. The cutoff is always the last argument. The energy of the wall potential is shifted so that the wall-particle interaction energy is 0.0 at the cutoff distance.

For a full description of these wall styles, see fix_style *wall*

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*.

The *fix_modify energy* option is supported by this fix to add the energy of interaction between atoms and the wall to the system's potential energy as part of *thermodynamic output*.

The *fix_modify virial* option is supported by this fix to add the contribution due to the interaction between atoms and each wall to the system's virial as part of *thermodynamic output*. The default is *virial no*

The *fix_modify respa* option is supported by this fix. This allows to set at which level of the *r-RESPA* integrator the fix is adding its forces. Default is the outermost level.

This fix computes a global scalar energy and a global 3-length vector of forces, which can be accessed by various *output commands*. The scalar energy is the sum of energy interactions for all particles interacting with the wall represented by the region surface. The 3 vector quantities are the x,y,z components of the total force acting on the wall due to the particles. The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command.

Note: If you want the atom/wall interaction energy to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the *fix_modify* *energy* option for this fix.

16.266.4 Restrictions

none

16.266.5 Related commands

fix wall/lj93, *fix wall/lj126*, *fix wall/lj1043*, *fix wall/colloid*, *fix wall/harmonic*, *fix wall/gran*

Default: none

16.267 fix wall/srd command

16.267.1 Syntax

```
fix ID group-ID wall/srd face arg ... keyword value ...
```

- ID, group-ID are documented in *fix* command
- wall/srd = style name of this fix command
- one or more face/arg pairs may be appended
- face = *xlo* or *xhi* or *ylo* or *yhi* or *zlo* or *zhi*

```
xlo,ylo,zlo arg = EDGE or constant or variable
  EDGE = current lo edge of simulation box
  constant = number like 0.0 or -30.0 (distance units)
  variable = equal-style variable like v_x or v_wiggle
xhi,yhi,zhi arg = EDGE or constant or variable
  EDGE = current hi edge of simulation box
  constant = number like 50.0 or 100.3 (distance units)
  variable = equal-style variable like v_x or v_wiggle
```

- zero or more keyword/value pairs may be appended
- keyword = *units*

```
units value = lattice or box
  lattice = the wall position is defined in lattice units
  box = the wall position is defined in simulation box units
```

16.267.2 Examples

```
fix xwalls all wall/srd xlo EDGE xhi EDGE
fix walls all wall/srd xlo 0.0 ylo 10.0 units box
fix top all wall/srd zhi v_pressdown
```

16.267.3 Description

Bound the simulation with one or more walls which interact with stochastic reaction dynamics (SRD) particles as slip (smooth) or no-slip (rough) flat surfaces. The wall interaction is actually invoked via the *fix srd* command, only on the group of SRD particles it defines, so the group setting for the fix wall/srd command is ignored.

A particle/wall collision occurs if an SRD particle moves outside the wall on a timestep. This alters the position and velocity of the SRD particle and imparts a force to the wall.

The *collision* and *Tsrd* settings specified via the *fix srd* command affect the SRD/wall collisions. A *slip* setting for the *collision* keyword means that the tangential component of the SRD particle momentum is preserved. Thus only a normal force is imparted to the wall. The normal component of the new SRD velocity is sampled from a Gaussian distribution at temperature *Tsrd*.

For a *noslip* setting of the *collision* keyword, both the normal and tangential components of the new SRD velocity are sampled from a Gaussian distribution at temperature *Tsrd*. Additionally, a new tangential direction for the SRD velocity is chosen randomly. This collision style imparts both a normal and tangential force to the wall.

Up to 6 walls or faces can be specified in a single command: *xlo*, *xhi*, *ylo*, *yhi*, *zlo*, *zhi*. A *lo* face reflects particles that move to a coordinate less than the wall position, back in the *hi* direction. A *hi* face reflects particles that move to a coordinate higher than the wall position, back in the *lo* direction.

The position of each wall can be specified in one of 3 ways: as the EDGE of the simulation box, as a constant value, or as a variable. If EDGE is used, then the corresponding boundary of the current simulation box is used. If a numeric constant is specified then the wall is placed at that position in the appropriate dimension (x, y, or z). In both the EDGE and constant cases, the wall will never move. If the wall position is a variable, it should be specified as v_name, where name is an *equal-style variable* name. In this case the variable is evaluated each timestep and the result becomes the current position of the reflecting wall. Equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent wall position.

Note: Because the trajectory of the SRD particle is tracked as it collides with the wall, you must insure that r = distance of the particle from the wall, is always > 0 for SRD particles, or LAMMPS will generate an error. This means you cannot start your simulation with SRD particles at the wall position *coord* (r = 0) or with particles on the wrong side of the wall (r < 0).

Note: If you have 2 or more walls that come together at an edge or corner (e.g. walls in the x and y dimensions), then be sure to set the *overlap* keyword to *yes* in the *fix srd* command, since the walls effectively overlap when SRD particles collide with them. LAMMPS will issue a warning if you do not do this.

Note: The walls of this fix only interact with SRD particles, as defined by the *fix srd* command. If you are simulating a mixture containing other kinds of particles, then you should typically use *another wall command* to act on the other particles. Since SRD particles will be colliding both with the walls and the other particles, it is important to insure that the other particle's finite extent does not overlap an SRD wall. If you do not do this, you may generate errors when SRD particles end up "inside" another particle or a wall at the beginning of a collision step.

The *units* keyword determines the meaning of the distance units used to define a wall position, but only when a numeric constant is used. It is not relevant when EDGE or a variable is used to specify a face position.

A *box* value selects standard distance units as defined by the *units* command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacings.

Here are examples of variable definitions that move the wall position in a time-dependent fashion using equal-style *variables*.

```
variable ramp equal ramp(0,10)
fix 1 all wall/srd xlo v_ramp

variable linear equal vdisplace(0,20)
fix 1 all wall/srd xlo v_linear

variable wiggle equal swiggle(0.0,5.0,3.0)
fix 1 all wall/srd xlo v_wiggle

variable wiggle equal cwiggle(0.0,5.0,3.0)
fix 1 all wall/srd xlo v_wiggle
```

The ramp(lo,hi) function adjusts the wall position linearly from lo to hi over the course of a run. The displace(c0,velocity) function does something similar using the equation position = c0 + velocity*delta, where delta is the elapsed time.

The swiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation, where omega = 2 PI / period:

```
position = c0 + A sin(omega*delta)
```

The cwiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation, which will have an initial wall velocity of 0.0, and thus may impose a gentler perturbation on the particles:

```
position = c0 + A (1 - cos(omega*delta))
```

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to *binary restart files*. None of the *fix_modify* options are relevant to this fix.

This fix computes a global array of values which can be accessed by various *output commands*. The number of rows in the array is equal to the number of walls defined by the fix. The number of columns is 3, for the x,y,z components of force on each wall.

Note that an outward normal force on a wall will be a negative value for *lo* walls and a positive value for *hi* walls. The array values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during *energy minimization*.

16.267.4 Restrictions

Any dimension (xyz) that has an SRD wall must be non-periodic.

16.267.5 Related commands

fix srd

Default: none

CHAPTER

SEVENTEEN

COMPUTES

17.1 compute ackland/atom command

17.1.1 Syntax

```
compute ID group-ID ackland/atom keyword/value
```

- ID, group-ID are documented in *compute* command
- ackland/atom = style name of this compute command
- zero or more keyword/value pairs may be appended
- keyword = *legacy*

  legacy yes/no = use (*yes*) or do not use (*no*) legacy ackland algorithm implementation

17.1.2 Examples

```
compute 1 all ackland/atom
compute 1 all ackland/atom legacy yes
```

17.1.3 Description

Defines a computation that calculates the local lattice structure according to the formulation given in *(Ackland)*. Historically, LAMMPS had two, slightly different implementations of the algorithm from the paper. With the *legacy* keyword, it is possible to switch between the pre-2015 (*legacy yes*) and post-2015 implementation (*legacy no*). The post-2015 variant is the default.

In contrast to the *centro-symmetry parameter* this method is stable against temperature boost, because it is based not on the distance between particles but the angles. Therefore statistical fluctuations are averaged out a little more. A comparison with the Common Neighbor Analysis metric is made in the paper.

The result is a number which is mapped to the following different lattice structures:

- 0 = UNKNOWN
- 1 = BCC
- 2 = FCC
- 3 = HCP

- 4 = ICO

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (i.e. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently or to have multiple compute/dump commands, each of which computes this quantity.-

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

17.1.4 Restrictions

This compute is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

The per-atom vector values will be unitless since they are the integers defined above.

17.1.5 Related commands

compute centro/atom

17.1.6 Default

The keyword *legacy* defaults to *no*.

(Ackland) Ackland, Jones, Phys Rev B, 73, 054104 (2006).

17.2 compute adf command

17.2.1 Syntax

```
compute ID group-ID adf Nbin itype1 jtype1 ktype1 Rjinner1 Rjouter1 Rkinner1 Rkouter1␣
↪...
```

- ID, group-ID are documented in *compute* command
- adf = style name of this compute command
- Nbin = number of ADF bins
- itypeN = central atom type for Nth ADF histogram (see asterisk form below)
- jtypeN = J atom type for Nth ADF histogram (see asterisk form below)
- ktypeN = K atom type for Nth ADF histogram (see asterisk form below)
- RjinnerN = inner radius of J atom shell for Nth ADF histogram (distance units)
- RjouterN = outer radius of J atom shell for Nth ADF histogram (distance units)
- RkinnerN = inner radius of K atom shell for Nth ADF histogram (distance units)
- RkouterN = outer radius of K atom shell for Nth ADF histogram (distance units)

- zero or one keyword/value pairs may be appended
- keyword = *ordinate*

```
ordinate value = degree or radian or cosine
  Choose the ordinate parameter for the histogram
```

17.2.2 Examples

```
compute 1 fluid adf 32 1 1 1 0.0 1.2 0.0 1.2 &
                       1 1 2 0.0 1.2 0.0 1.5 &
                       1 2 2 0.0 1.5 0.0 1.5 &
                       2 1 1 0.0 1.2 0.0 1.2 &
                       2 1 2 0.0 1.5 2.0 3.5 &
                       2 2 2 2.0 3.5 2.0 3.5
compute 1 fluid adf 32 1*2 1*2 1*2 0.5 3.5
compute 1 fluid adf 32
```

17.2.3 Description

Define a computation that calculates one or more angular distribution functions (ADF) for a group of particles. Each ADF is calculated in histogram form by measuring the angle formed by a central atom and two neighbor atoms and binning these angles into *Nbin* bins. Only neighbors for which *Rinner* < *R* < *Router* are counted, where *Rinner* and *Router* are specified separately for the first and second neighbor atom in each requested ADF.

Note: If you have a bonded system, then the settings of *special_bonds* command can remove pairwise interactions between atoms in the same bond, angle, or dihedral. This is the default setting for the *special_bonds* command, and means those pairwise interactions do not appear in the neighbor list. Because this fix uses a neighbor list, it also means those pairs will not be included in the ADF. This does not apply when using long-range coulomb interactions (*coul/long*, *coul/msm*, *coul/wolf* or similar. One way to get around this would be to set special_bond scaling factors to very tiny numbers that are not exactly zero (e.g. 1.0e-50). Another workaround is to write a dump file, and use the *rerun* command to compute the ADF for snapshots in the dump file. The rerun script can use a *special_bonds* command that includes all pairs in the neighbor list.

Note: If you request any outer cutoff *Router* > force cutoff, or if no pair style is defined, e.g. the *rerun* command is being used to post-process a dump file of snapshots you must insure ghost atom information out to the largest value of *Router* + *skin* is communicated, via the *comm_modify cutoff* command, else the ADF computation cannot be performed, and LAMMPS will give an error message. The *skin* value is what is specified with the *neighbor* command.

The *itypeN*,*jtypeN*,*ktypeN* settings can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to specify a range of atom types as in the 2nd example above. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

If *itypeN*, *jtypeN*, and *ktypeN* are single values, as in the 1st example above, this means that the ADF is computed where atoms of type *itypeN* are the central atom, and neighbor atoms of type *jtypeN* and *ktypeN* are forming the angle. If any of *itypeN*, *jtypeN*, or *ktypeN* represent a range of values via the wild-card asterisk, as in the 2nd example above, this means that the ADF is computed where atoms of any of the range of types represented by *itypeN* are the central atom, and the angle is formed by two neighbors, one neighbor in the range of types represented by *jtypeN* and another neighbor in the range of types represented by *ktypeN*.

If no *itypeN*, *jtypeN*, *ktypeN* settings are specified, then LAMMPS will generate a single ADF for all atoms in the group. The inner cutoff is set to zero and the outer cutoff is set to the force cutoff. If no pair_style is specified, there is no force cutoff and LAMMPS will give an error message. Note that in most cases, generating an ADF for all atoms is not a good thing. Such an ADF is both uninformative and extremely expensive to compute. For example, with liquid water with a 10 A force cutoff, there are 80,000 angles per atom. In addition, most of the interesting angular structure occurs for neighbors that are the closest to the central atom, involving just a few dozen angles.

Angles for each ADF are generated by double-looping over the list of neighbors of each central atom I, just as they would be in the force calculation for a three-body potential such as *Stillinger-Weber*. The angle formed by central atom I and neighbor atoms J and K is included in an ADF if the following criteria are met:

- atoms I,J,K are all in the specified compute group
- the distance between atoms I,J is between Rjinner and Rjouter
- the distance between atoms I,K is between Rkinner and Rkouter
- the type of the I atom matches itypeN (one or a range of types)
- atoms I,J,K are distinct
- the type of the J atom matches jtypeN (one or a range of types)
- the type of the K atom matches ktypeN (one or a range of types)

Each unique angle satisfying the above criteria is counted only once, regardless of whether either or both of the neighbor atoms making up the angle appear in both the J and K lists. It is OK if a particular angle is included in more than one individual histogram, due to the way the *itypeN*, *jtypeN*, *ktypeN* arguments are specified.

The first ADF value for a bin is calculated from the histogram count by dividing by the total number of triples satisfying the criteria, so that the integral of the ADF w.r.t. angle is 1, i.e. the ADF is a probability density function.

The second ADF value is reported as a cumulative sum of all bins up to the current bins, averaged over atoms of type *itypeN*. It represents the number of angles per central atom with angle less than or equal to the angle of the current bin, analogous to the coordination number radial distribution function.

The *ordinate* optional keyword determines whether the bins are of uniform angular size from zero to 180 (*degree*), zero to Pi (*radian*), or the cosine of the angle uniform in the range [-1,1] (*cosine*). *cosine* has the advantage of eliminating the *acos()* function call, which speeds up the compute by 2-3x, and it is also preferred on physical grounds, because the for uniformly distributed particles in 3D, the angular probability density w.r.t dtheta is sin(theta)/2, while for d(cos(theta)), it is 1/2, Regardless of which ordinate is chosen, the first column of ADF values is normalized w.r.t. the range of that ordinate, so that the integral is 1.

The simplest way to output the results of the compute adf calculation to a file is to use the *fix ave/time* command, for example:

```
compute myADF all adf 32 2 2 2 0.5 3.5 0.5 3.5
fix 1 all ave/time 100 1 100 c_myADF[*] file tmp.adf mode vector
```

Output info:

This compute calculates a global array with the number of rows = *Nbins*, and the number of columns = 1 + 2*Ntriples, where Ntriples is the number of I,J,K triples specified. The first column has the bin coordinate (angle-related ordinate at midpoint of bin). Each subsequent column has the two ADF values for a specific set of (*itypeN*,*jtypeN*,*ktypeN*) interactions, as described above. These values can be used by any command that uses a global values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The array values calculated by this compute are all "intensive".

The first column of array values is the angle-related ordinate, either the angle in degrees or radians, or the cosine of the angle. Each subsequent pair of columns gives the first and second kinds of ADF for a specific set of (*itypeN*,*jtypeN*,*ktypeN*). The values in the first ADF column are normalized numbers >= 0.0, whose integral w.r.t. the ordinate is 1, i.e. the first ADF is a normalized probability distribution. The values in the second ADF column are also

numbers >= 0.0. They are the cumulative density distribution of angles per atom. By definition, this ADF is monotonically increasing from zero to a maximum value equal to the average total number of angles per atom satisfying the ADF criteria.

17.2.4 Restrictions

The ADF is not computed for neighbors outside the force cutoff, since processors (in parallel) don't know about atom coordinates for atoms further away than that distance. If you want an ADF for larger distances, you can use the *rerun* command to post-process a dump file and set the cutoff for the potential to be longer in the rerun script. Note that in the rerun context, the force cutoff is arbitrary, since you aren't running dynamics and thus are not changing your model.

17.2.5 Related commands

compute rdf, *fix ave/time*, *compute_modify*

17.2.6 Default

The keyword default is ordinate = degree.

17.3 compute angle command

17.3.1 Syntax

```
compute ID group-ID angle
```

- ID, group-ID are documented in *compute* command
- angle = style name of this compute command

17.3.2 Examples

```
compute 1 all angle
```

17.3.3 Description

Define a computation that extracts the angle energy calculated by each of the angle sub-styles used in the "angle_style hybrid" angle_hybrid.html command. These values are made accessible for output or further processing by other commands. The group specified for this command is ignored.

This compute is useful when using *angle_style hybrid* if you want to know the portion of the total energy contributed by one or more of the hybrid sub-styles.

Output info:

This compute calculates a global vector of length N where N is the number of sub_styles defined by the *angle_style hybrid* command, which can be accessed by indices 1-N. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector values are "extensive" and will be in energy *units*.

17.3.4 Restrictions

none

17.3.5 Related commands

compute pe, *compute pair*

Default: none

17.4 compute angle/local command

17.4.1 Syntax

```
compute ID group-ID angle/local value1 value2 ... keyword args ...
```

- ID, group-ID are documented in *compute* command
- angle/local = style name of this compute command
- one or more values may be appended
- value = *theta* or *eng* or *v_name*

```
theta = tabulate angles
eng = tabulate angle energies
v_name = equal-style variable with name (see below)
```

- zero or more keyword/args pairs may be appended
- keyword = *set*

```
set args = theta name
  theta = only currently allowed arg
  name = name of variable to set with theta
```

17.4.2 Examples

```
compute 1 all angle/local theta
compute 1 all angle/local eng theta
compute 1 all angle/local theta v_cos set theta t
```

17.4.3 Description

Define a computation that calculates properties of individual angle interactions. The number of datums generated, aggregated across all processors, equals the number of angles in the system, modified by the group parameter as explained below.

The value *theta* is the angle for the 3 atoms in the interaction.

The value *eng* is the interaction energy for the angle.

The value *v_name* can be used together with the *set* keyword to compute a user-specified function of the angle theta. The *name* specified for the *v_name* value is the name of an *equal-style variable* which should evaluate a formula based on a variable which will store the angle theta. This other variable must be an *internal-style variable* defined in the input script; its initial numeric value can be anything. It must be an internal-style variable, because this command resets its value directly. The *set* keyword is used to identify the name of this other variable associated with theta.

Note that the value of theta for each angle which stored in the internal variable is in radians, not degrees.

As an example, these commands can be added to the bench/in.rhodo script to compute the cosine and cosine^2 of every angle in the system and output the statistics in various ways:

```
variable t internal 0.0
variable cos equal cos(v_t)
variable cossq equal cos(v_t)*cos(v_t)

compute 1 all property/local aatom1 aatom2 aatom3 atype
compute 2 all angle/local eng theta v_cos v_cossq set theta t
dump 1 all local 100 tmp.dump c_1[*] c_2[*]

compute 3 all reduce ave c_2[*]
thermo_style custom step temp press c_3[*]

fix 10 all ave/histo 10 10 100 -1 1 20 c_2[3] mode vector file tmp.histo
```

The *dump local* command will output the energy, angle, cosine(angle), cosine^2(angle) for every angle in the system. The *thermo_style* command will print the average of those quantities via the *compute reduce* command with thermo output. And the *fix ave/histo* command will histogram the cosine(angle) values and write them to a file.

The local data stored by this command is generated by looping over all the atoms owned on a processor and their angles. An angle will only be included if all 3 atoms in the angle are in the specified compute group. Any angles that have been broken (see the *angle_style* command) by setting their angle type to 0 are not included. Angles that have been turned off (see the *fix shake* or *delete_bonds* commands) by setting their angle type negative are written into the file, but their energy will be 0.0.

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For example, angle output from the *compute property/local* command can be combined with data from this command and output by the *dump local* command in a consistent way.

Here is an example of how to do this:

```
compute 1 all property/local atype aatom1 aatom2 aatom3
compute 2 all angle/local theta eng
dump 1 all local 1000 tmp.dump index c_1[1] c_1[2] c_1[3] c_1[4] c_2[1] c_2[2]
```

Output info:

This compute calculates a local vector or local array depending on the number of values. The length of the vector or number of rows in the array is the number of angles. If a single value is specified, a local vector is produced. If two or more values are specified, a local array is produced where the number of columns = the number of values. The vector or array can be accessed by any command that uses local values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The output for *theta* will be in degrees. The output for *eng* will be in energy *units*.

17.4.4 Restrictions

none

17.4.5 Related commands

dump local, *compute property/local*

Default: none

17.5 compute angmom/chunk command

17.5.1 Syntax

```
compute ID group-ID angmom/chunk chunkID
```

- ID, group-ID are documented in *compute* command
- angmom/chunk = style name of this compute command
- chunkID = ID of *compute chunk/atom* command

17.5.2 Examples

```
compute 1 fluid angmom/chunk molchunk
```

17.5.3 Description

Define a computation that calculates the angular momentum of multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a *compute chunk/atom* command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the *compute chunk/atom* and *Howto chunk* doc pages for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

This compute calculates the 3 components of the angular momentum vector for each chunk, due to the velocity/momentum of the individual atoms in the chunk around the center-of-mass of the chunk. The calculation includes all effects due to atoms passing through periodic boundaries.

Note that only atoms in the specified group contribute to the calculation. The *compute chunk/atom* command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

Note: The coordinates of an atom contribute to the chunk's angular momentum in "unwrapped" form, by using the image flags associated with each atom. See the *dump custom* command for a discussion of "unwrapped" coordinates. See the Atoms section of the *read_data* command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the *set image* command.

The simplest way to output the results of the compute angmom/chunk calculation to a file is to use the *fix ave/time* command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all angmom/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk[*] file tmp.out mode vector
```

Output info:

This compute calculates a global array where the number of rows = the number of chunks *Nchunk* as calculated by the specified *compute chunk/atom* command. The number of columns = 3 for the 3 xyz components of the angular momentum for each chunk. These values can be accessed by any command that uses global array values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The array values are "intensive". The array values will be in mass-velocity-distance *units*.

17.5.4 Restrictions

none

17.5.5 Related commands

variable angmom() function

Default: none

17.6 compute basal/atom command

17.6.1 Syntax

```
compute ID group-ID basal/atom
```

- ID, group-ID are documented in *compute* command
- basal/atom = style name of this compute command

17.6.2 Examples

```
compute 1 all basal/atom
```

17.6.3 Description

Defines a computation that calculates the hexagonal close-packed "c" lattice vector for each atom in the group. It does this by calculating the normal unit vector to the basal plane for each atom. The results enable efficient identification and characterization of twins and grains in hexagonal close-packed structures.

The output of the compute is thus the 3 components of a unit vector associated with each atom. The components are set to 0.0 for atoms not in the group.

Details of the calculation are given in *(Barrett)*.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (i.e. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently or to have multiple compute/dump commands, each of which computes this quantity.

An example input script that uses this compute is provided in examples/USER/misc/basal.

Output info:

This compute calculates a per-atom array with 3 columns, which can be accessed by indices 1-3 by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values are unitless since the 3 columns represent components of a unit vector.

17.6.4 Restrictions

This compute is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

The output of this compute will be meaningless unless the atoms are on (or near) hcp lattice sites, since the calculation assumes a well-defined basal plane.

17.6.5 Related commands

compute centro/atom, *compute ackland/atom*

Default: none

(Barrett) Barrett, Tschopp, El Kadiri, Scripta Mat. 66, p.666 (2012).

17.7 compute body/local command

17.7.1 Syntax

```
compute ID group-ID body/local input1 input2 ...
```

- ID, group-ID are documented in *compute* command
- body/local = style name of this compute command
- one or more keywords may be appended
- keyword = *id* or *type* or *integer*

```
id = atom ID of the body particle
type = atom type of the body particle
integer = 1,2,3,etc = index of fields defined by body style
```

17.7.2 Examples

```
compute 1 all body/local type 1 2 3
compute 1 all body/local 3 6
```

17.7.3 Description

Define a computation that calculates properties of individual body sub-particles. The number of datums generated, aggregated across all processors, equals the number of body sub-particles plus the number of non-body particles in the system, modified by the group parameter as explained below. See the *Howto body* doc page for more details on using body particles.

The local data stored by this command is generated by looping over all the atoms. An atom will only be included if it is in the group. If the atom is a body particle, then its N sub-particles will be looped over, and it will contribute N datums to the count of datums. If it is not a body particle, it will contribute 1 datum.

For both body particles and non-body particles, the *id* keyword will store the ID of the particle.

For both body particles and non-body particles, the *type* keyword will store the type of the particle.

The *integer* keywords mean different things for body and non-body particles. If the atom is not a body particle, only its x, y, z coordinates can be referenced, using the *integer* keywords 1,2,3. Note that this means that if you want to access more fields than this for body particles, then you cannot include non-body particles in the group.

For a body particle, the *integer* keywords refer to fields calculated by the body style for each sub-particle. The body style, as specified by the *atom_style body*, determines how many fields exist and what they are. See the *Howto_body* doc page for details of the different styles.

Here is an example of how to output body information using the *dump local* command with this compute. If fields 1,2,3 for the body sub-particles are x,y,z coordinates, then the dump file will be formatted similar to the output of a *dump atom or custom* command.

```
compute 1 all body/local type 1 2 3
dump 1 all local 1000 tmp.dump index c_1[1] c_1[2] c_1[3] c_1[4]
```

Output info:

This compute calculates a local vector or local array depending on the number of keywords. The length of the vector or number of rows in the array is the number of datums as described above. If a single keyword is specified, a local vector is produced. If two or more keywords are specified, a local array is produced where the number of columns = the number of keywords. The vector or array can be accessed by any command that uses local values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The *units* for output values depend on the body style.

17.7.4 Restrictions

none

17.7.5 Related commands

dump local

Default: none

17.8 compute bond command

17.8.1 Syntax

```
compute ID group-ID bond
```

- ID, group-ID are documented in *compute* command
- bond = style name of this compute command

17.8.2 Examples

```
compute 1 all bond
```

17.8.3 Description

Define a computation that extracts the bond energy calculated by each of the bond sub-styles used in the *bond_style hybrid* command. These values are made accessible for output or further processing by other commands. The group specified for this command is ignored.

This compute is useful when using *bond_style hybrid* if you want to know the portion of the total energy contributed by one or more of the hybrid sub-styles.

Output info:

This compute calculates a global vector of length N where N is the number of sub_styles defined by the *bond_style hybrid* command, which can be accessed by indices 1-N. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector values are "extensive" and will be in energy *units*.

17.8.4 Restrictions

none

17.8.5 Related commands

compute pe, *compute pair*

Default: none

17.9 compute bond/local command

17.9.1 Syntax

```
compute ID group-ID bond/local value1 value2 ... keyword args ...
```

- ID, group-ID are documented in *compute* command
- bond/local = style name of this compute command
- one or more values may be appended
- value = *dist* or *engpot* or *force* or *fx* or *fy* or *fz* or *engvib* or *engrot* or *engtrans* or *omega* or *velvib* or *v_name*

```
dist = bond distance
engpot = bond potential energy
force = bond force

fx,fy,fz = components of bond force
engvib = bond kinetic energy of vibration
engrot = bond kinetic energy of rotation
engtrans = bond kinetic energy of translation
omega = magnitude of bond angular velocity
velvib = vibrational velocity along the bond length
v_name = equal-style variable with name (see below)
```

- zero or more keyword/args pairs may be appended
- keyword = *set*

```
set args = dist name
  dist = only currently allowed arg
  name = name of variable to set with distance (dist)
```

17.9.2 Examples

```
compute 1 all bond/local engpot
compute 1 all bond/local dist engpot force

compute 1 all bond/local dist fx fy fz

compute 1 all angle/local dist v_distsq set dist d
```

17.9.3 Description

Define a computation that calculates properties of individual bond interactions. The number of datums generated, aggregated across all processors, equals the number of bonds in the system, modified by the group parameter as explained below.

All these properties are computed for the pair of atoms in a bond, whether the 2 atoms represent a simple diatomic molecule, or are part of some larger molecule.

The value *dist* is the current length of the bond.

The value *engpot* is the potential energy for the bond, based on the current separation of the pair of atoms in the bond.

The value *force* is the magnitude of the force acting between the pair of atoms in the bond.

The values *fx*, *fy*, and *fz* are the xyz components of *force* between the pair of atoms in the bond.

The remaining properties are all computed for motion of the two atoms relative to the center of mass (COM) velocity of the 2 atoms in the bond.

The value *engvib* is the vibrational kinetic energy of the two atoms in the bond, which is simply 1/2 m1 v1^2 + 1/2 m2 v2^2, where v1 and v2 are the magnitude of the velocity of the 2 atoms along the bond direction, after the COM velocity has been subtracted from each.

The value *engrot* is the rotational kinetic energy of the two atoms in the bond, which is simply 1/2 m1 v1^2 + 1/2 m2 v2^2, where v1 and v2 are the magnitude of the velocity of the 2 atoms perpendicular to the bond direction, after the COM velocity has been subtracted from each.

The value *engtrans* is the translational kinetic energy associated with the motion of the COM of the system itself, namely 1/2 (m1+m2) Vcm^2 where Vcm = magnitude of the velocity of the COM.

Note that these 3 kinetic energy terms are simply a partitioning of the summed kinetic energy of the 2 atoms themselves. I.e. total KE = 1/2 m1 v1^2 + 1/2 m2 v2^2 = engvib + engrot + engtrans, where v1,v2 are the magnitude of the velocities of the 2 atoms, without any adjustment for the COM velocity.

The value *omega* is the magnitude of the angular velocity of the two atoms around their COM position.

The value *velvib* is the magnitude of the relative velocity of the two atoms in the bond towards each other. A negative value means the 2 atoms are moving toward each other; a positive value means they are moving apart.

The value *v_name* can be used together with the *set* keyword to compute a user-specified function of the bond distance. The *name* specified for the *v_name* value is the name of an *equal-style variable* which should evaluate a formula based on a variable which will store the bond distance. This other variable must be an *internal-style variable* defined in the input script; its initial numeric value can be anything. It must be an internal-style variable, because this command resets its value directly. The *set* keyword is used to identify the name of this other variable associated with theta.

As an example, these commands can be added to the bench/in.rhodo script to compute the distance^2 of every bond in the system and output the statistics in various ways:

```
variable d internal 0.0
variable dsq equal v_d*v_d

compute 1 all property/local batom1 batom2 btype
compute 2 all bond/local engpot dist v_dsq set dist d
dump 1 all local 100 tmp.dump c_1[*] c_2[*]

compute 3 all reduce ave c_2[*]
thermo_style custom step temp press c_3[*]

fix 10 all ave/histo 10 10 100 0 6 20 c_2[3] mode vector file tmp.histo
```

The *dump local* command will output the energy, distance, distance^2 for every bond in the system. The *thermo_style* command will print the average of those quantities via the *compute reduce* command with thermo output. And the *fix ave/histo* command will histogram the distance^2 values and write them to a file.

The local data stored by this command is generated by looping over all the atoms owned on a processor and their bonds. A bond will only be included if both atoms in the bond are in the specified compute group. Any bonds that have been broken (see the *bond_style* command) by setting their bond type to 0 are not included. Bonds that have been turned off (see the *fix shake* or *delete_bonds* commands) by setting their bond type negative are written into the file, but their energy will be 0.0.

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For example, bond output from the *compute property/local* command can be combined with data from this command and output by the *dump local* command in a consistent way.

Here is an example of how to do this:

```
compute 1 all property/local btype batom1 batom2
compute 2 all bond/local dist engpot
dump 1 all local 1000 tmp.dump index c_1[*] c_2[*]
```

Output info:

This compute calculates a local vector or local array depending on the number of values. The length of the vector or number of rows in the array is the number of bonds. If a single value is specified, a local vector is produced. If two or more values are specified, a local array is produced where the number of columns = the number of values. The vector or array can be accessed by any command that uses local values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The output for *dist* will be in distance *units*. The output for *velvib* will be in velocity *units*. The output for *omega* will be in velocity/distance *units*. The output for *engtrans*, *engvib*, *engrot*, and *engpot* will be in energy *units*. The output for *force* will be in force *units*.

17.9.4 Restrictions

none

17.9.5 Related commands

dump local, *compute property/local*

Default: none

17.10 compute centro/atom command

17.10.1 Syntax

```
compute ID group-ID centro/atom lattice keyword value ...
```

- ID, group-ID are documented in *compute* command centro/atom = style name of this compute command lattice = *fcc* or *bcc* or N = # of neighbors per atom to include

- zero or more keyword/value pairs may be appended
- keyword = *axes*

```
axes value = no or yes
  no = do not calculate 3 symmetry axes
  yes = calculate 3 symmetry axes
```

17.10.2 Examples

```
compute 1 all centro/atom fcc

compute 1 all centro/atom 8
```

17.10.3 Description

Define a computation that calculates the centro-symmetry parameter for each atom in the group, for either FCC or BCC lattices, depending on the choice of the *lattice* argument. In solid-state systems the centro-symmetry parameter is a useful measure of the local lattice disorder around an atom and can be used to characterize whether the atom is part of a perfect lattice, a local defect (e.g. a dislocation or stacking fault), or at a surface.

The value of the centro-symmetry parameter will be 0.0 for atoms not in the specified compute group.

This parameter is computed using the following formula from *(Kelchner)*

$$CS = \sum_{i=1}^{N/2} |\vec{R}_i + \vec{R}_{i+N/2}|^2$$

where the N nearest neighbors of each atom are identified and $\vec{R}_i$ and $\vec{R}_{i+N/2}$ are vectors from the central atom to a particular pair of nearest neighbors. There are $N(N-1)/2$ possible neighbor pairs that can contribute to this formula. The quantity in the sum is computed for each, and the $N/2$ smallest are used. This will typically be for pairs of atoms in symmetrically opposite positions with respect to the central atom; hence the $i + N/2$ notation.

N is an input parameter, which should be set to correspond to the number of nearest neighbors in the underlying lattice of atoms. If the keyword *fcc* or *bcc* is used, *N* is set to 12 and 8 respectively. More generally, *N* can be set to a positive, even integer.

For an atom on a lattice site, surrounded by atoms on a perfect lattice, the centro-symmetry parameter will be 0. It will be near 0 for small thermal perturbations of a perfect lattice. If a point defect exists, the symmetry is broken, and the parameter will be a larger positive value. An atom at a surface will have a large positive parameter. If the atom does not have N neighbors (within the potential cutoff), then its centro-symmetry parameter is set to 0.0.

If the keyword *axes* has the setting *yes*, then this compute also estimates three symmetry axes for each atom's local neighborhood. The first two of these are the vectors joining the two pairs of neighbor atoms with smallest contributions to the centrosymmetry parameter, i.e. the two most symmetric pairs of atoms. The third vector is normal to the first two by the right-hand rule. All three vectors are normalized to unit length. For FCC crystals, the first two vectors will lie along a <110> direction, while the third vector will lie along either a <100> or <111> direction. For HCP crystals, the first two vectors will lie along <1000> directions, while the third vector will lie along <0001>. This provides a simple way to measure local orientation in HCP structures. In general, the *axes* keyword can be used to estimate the orientation of symmetry axes in the neighborhood of any atom.

Only atoms within the cutoff of the pairwise neighbor list are considered as possible neighbors. Atoms not in the compute group are included in the N neighbors used in this calculation.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (e.g. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently or to have multiple compute/dump commands, each with a *centro/atom* style.

Output info:

By default, this compute calculates the centrosymmetry value for each atom as a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

If the *axes* keyword setting is *yes*, then a per-atom array is calculated. The first column is the centrosymmetry parameter. The next three columns are the x, y, and z components of the first symmetry axis, followed by the second, and third symmetry axes in columns 5-7 and 8-10.

The centrosymmetry values are unitless values >= 0.0. Their magnitude depends on the lattice style due to the number of contributing neighbor pairs in the summation in the formula above. And it depends on the local defects surrounding the central atom, as described above. For the *axes yes* case, the vector components are also unitless, since they represent spatial directions.

Here are typical centro-symmetry values, from a nanoindentation simulation into gold (FCC). These were provided by Jon Zimmerman (Sandia):

```
Bulk lattice = 0
Dislocation core ~ 1.0 (0.5 to 1.25)
Stacking faults ~ 5.0 (4.0 to 6.0)
Free surface ~ 23.0
```

These values are *not* normalized by the square of the lattice parameter. If they were, normalized values would be:

```
Bulk lattice = 0
Dislocation core ~ 0.06 (0.03 to 0.075)
Stacking faults ~ 0.3 (0.24 to 0.36)
Free surface ~ 1.38
```

For BCC materials, the values for dislocation cores and free surfaces would be somewhat different, due to their being only 8 neighbors instead of 12.

17.10.4 Restrictions

none

17.10.5 Related commands

compute cna/atom

17.10.6 Default

The default value for the optional keyword is axes = no.

(Kelchner) Kelchner, Plimpton, Hamilton, Phys Rev B, 58, 11085 (1998).

17.11 compute chunk/atom command

17.11.1 Syntax

```
compute ID group-ID chunk/atom style args keyword values ...
```

- ID, group-ID are documented in *compute* command
- chunk/atom = style name of this compute command

```
style = bin/1d or bin/2d or bin/3d or bin/sphere or type or molecule or␣
↪c_ID, c_ID[I], f_ID, f_ID[I], v_name
  bin/1d args = dim origin delta
    dim = x or y or z
    origin = lower or center or upper or coordinate value (distance␣
↪units)
    delta = thickness of spatial bins in dim (distance units)
  bin/2d args = dim origin delta dim origin delta
    dim = x or y or z
    origin = lower or center or upper or coordinate value (distance␣
↪units)
    delta = thickness of spatial bins in dim (distance units)
  bin/3d args = dim origin delta dim origin delta dim origin delta
    dim = x or y or z
    origin = lower or center or upper or coordinate value (distance␣
↪units)
    delta = thickness of spatial bins in dim (distance units)
  bin/sphere args = xorig yorig zorig rmin rmax nsbin
    xorig,yorig,zorig = center point of sphere
    srmin,srmax = bin from sphere radius rmin to rmax
    nsbin = # of spherical shell bins between rmin and rmax
  bin/cylinder args = dim origin delta c1 c2 rmin rmax ncbin
    dim = x or y or z = axis of cylinder axis
    origin = lower or center or upper or coordinate value (distance␣
↪units)
    delta = thickness of spatial bins in dim (distance units)
    c1,c2 = coords of cylinder axis in other 2 dimensions (distance units)
    crmin,crmax = bin from cylinder radius rmin to rmax (distance units)
    ncbin = # of concentric circle bins between rmin and rmax
  type args = none
  molecule args = none
  c_ID, c_ID[I], f_ID, f_ID[I], v_name args = none
    c_ID = per-atom vector calculated by a compute with ID
    c_ID[I] = Ith column of per-atom array calculated by a compute with ID
    f_ID = per-atom vector calculated by a fix with ID
    f_ID[I] = Ith column of per-atom array calculated by a fix with ID
    v_name = per-atom vector calculated by an atom-style variable with␣
↪name
```

- zero or more keyword/values pairs may be appended
- keyword = *region* or *nchunk* or *static* or *compress* or *bound* or *discard* or *pbc* or *units*

```
region value = region-ID
  region-ID = ID of region atoms must be in to be part of a chunk
```

```
nchunk value = once or every
  once = only compute the number of chunks once
  every = re-compute the number of chunks whenever invoked
limit values = 0 or Nc max or Nc exact
  0 = no limit on the number of chunks
  Nc max = limit number of chunks to be <= Nc
  Nc exact = set number of chunks to exactly Nc
ids value = once or nfreq or every
  once = assign chunk IDs to atoms only once, they persist thereafter
  nfreq = assign chunk IDs to atoms only once every Nfreq steps (if␣
↪invoked by fix ave/chunk which sets Nfreq)
  every = assign chunk IDs to atoms whenever invoked
compress value = yes or no
  yes = compress chunk IDs to eliminate IDs with no atoms
  no = do not compress chunk IDs even if some IDs have no atoms
discard value = yes or no or mixed
  yes = discard atoms with out-of-range chunk IDs by assigning a chunk ID␣
↪= 0
  no = keep atoms with out-of-range chunk IDs by assigning a valid chunk␣
↪ID
  mixed = keep or discard such atoms according to spatial binning rule
bound values = x/y/z lo hi
  x/y/z = x or y or z to bound sptial bins in this dimension
  lo = lower or coordinate value (distance units)
  hi = upper or coordinate value (distance units)
pbc value = no or yes
  yes = use periodic distance for bin/sphere and bin/cylinder styles
units value = box or lattice or reduced
```

17.11.2 Examples

```
compute 1 all chunk/atom type
compute 1 all chunk/atom bin/1d z lower 0.02 units reduced
compute 1 all chunk/atom bin/2d z lower 1.0 y 0.0 2.5
compute 1 all chunk/atom molecule region sphere nchunk once ids once compress yes
compute 1 all chunk/atom bin/sphere 5 5 5 2.0 5.0 5 discard yes
compute 1 all chunk/atom bin/cylinder z lower 2 10 10 2.0 5.0 3 discard yes
compute 1 all chunk/atom c_cluster
```

17.11.3 Description

Define a computation that calculates an integer chunk ID from 1 to Nchunk for each atom in the group. Values of chunk IDs are determined by the *style* of chunk, which can be based on atom type or molecule ID or spatial binning or a per-atom property or value calculated by another *compute*, *fix*, or *atom-style variable*. Per-atom chunk IDs can be used by other computes with "chunk" in their style name, such as *compute com/chunk* or *compute msd/chunk*. Or they can be used by the *fix ave/chunk* command to sum and time average a variety of per-atom properties over the atoms in each chunk. Or they can simply be accessed by any command that uses per-atom values from a compute as input, as discussed on the *Howto output* doc page.

See the *Howto chunk* doc page for an overview of how this compute can be used with a variety of other commands to tabulate properties of a simulation. The page gives several examples of input script commands that can be used to calculate interesting properties.

Conceptually it is important to realize that this compute does two simple things. First, it sets the value of *Nchunk* = the number of chunks, which can be a constant value or change over time. Second, it assigns each atom to a chunk via a chunk ID. Chunk IDs range from 1 to *Nchunk* inclusive; some chunks may have no atoms assigned to them. Atoms that do not belong to any chunk are assigned a value of 0. Note that the two operations are not always performed together. For example, spatial bins can be setup once (which sets *Nchunk*), and atoms assigned to those bins many times thereafter (setting their chunk IDs).

All other commands in LAMMPS that use chunk IDs assume there are *Nchunk* number of chunks, and that every atom is assigned to one of those chunks, or not assigned to any chunk.

There are many options for specifying for how and when *Nchunk* is calculated, and how and when chunk IDs are assigned to atoms. The details depend on the chunk *style* and its *args*, as well as optional keyword settings. They can also depend on whether a *fix ave/chunk* command is using this compute, since that command requires *Nchunk* to remain static across windows of timesteps it specifies, while it accumulates per-chunk averages.

The details are described below.

The different chunk styles operate as follows. For each style, how it calculates *Nchunk* and assigns chunk IDs to atoms is explained. Note that using the optional keywords can change both of those actions, as described further below where the keywords are discussed.

The *binning* styles perform a spatial binning of atoms, and assign an atom the chunk ID corresponding to the bin number it is in. *Nchunk* is set to the number of bins, which can change if the simulation box size changes. This also depends on the setting of the *units* keyword; e.g. for *reduced* units the number of chunks may not change even if the box size does.

The *bin/1d*, *bin/2d*, and *bin/3d* styles define bins as 1d layers (slabs), 2d pencils, or 3d boxes. The *dim*, *origin*, and *delta* settings are specified 1, 2, or 3 times. For 2d or 3d bins, there is no restriction on specifying dim = x before dim = y or z, or dim = y before dim = z. Bins in a particular *dim* have a bin size in that dimension given by *delta*. In each dimension, bins are defined relative to a specified *origin*, which may be the lower/upper edge of the simulation box (in that dimension), or its center point, or a specified coordinate value. Starting at the origin, sufficient bins are created in both directions to completely span the simulation box or the bounds specified by the optional *bounds* keyword.

For orthogonal simulation boxes, the bins are layers, pencils, or boxes aligned with the xyz coordinate axes. For triclinic (non-orthogonal) simulation boxes, the bin faces are parallel to the tilted faces of the simulation box. See the *Howto triclinic* doc page for a discussion of the geometry of triclinic boxes in LAMMPS. As described there, a tilted simulation box has edge vectors a,b,c. In that nomenclature, bins in the x dimension have faces with normals in the "b" cross "c" direction. Bins in y have faces normal to the "a" cross "c" direction. And bins in z have faces normal to the "a" cross "b" direction. Note that in order to define the size and position of these bins in an unambiguous fashion, the *units* option must be set to *reduced* when using a triclinic simulation box, as noted below.

The meaning of *origin* and *delta* for triclinic boxes is as follows. Consider a triclinic box with bins that are 1d layers or slabs in the x dimension. No matter how the box is tilted, an *origin* of 0.0 means start layers at the lower "b" cross "c" plane of the simulation box and an *origin* of 1.0 means to start layers at the upper "b" cross "c" face of the box. A *delta* value of 0.1 in *reduced* units means there will be 10 layers from 0.0 to 1.0, regardless of the current size or shape of the simulation box.

The *bin/sphere* style defines a set of spherical shell bins around the origin (*xorig*,*yorig*,*zorig*), using *nsbin* bins with radii equally spaced between *srmin* and *srmax*. This is effectively a 1d vector of bins. For example, if *srmin* = 1.0 and *srmax* = 10.0 and *nsbin* = 9, then the first bin spans 1.0 < r < 2.0, and the last bin spans 9.0 < r 10.0. The geometry of the bins is the same whether the simulation box is orthogonal or triclinic; i.e. the spherical shells are not tilted or scaled differently in different dimensions to transform them into ellipsoidal shells.

The *bin/cylinder* style defines bins for a cylinder oriented along the axis *dim* with the axis coordinates in the other two radial dimensions at (*c1*,*c2*). For dim = x, c1/c2 = y/z; for dim = y, c1/c2 = x/z; for dim = z, c1/c2 = x/y. This is effectively a 2d array of bins. The first dimension is along the cylinder axis, the second dimension is radially outward

from the cylinder axis. The bin size and positions along the cylinder axis are specified by the *origin* and *delta* values, the same as for the *bin/1d*, *bin/2d*, and *bin/3d* styles. There are *ncbin* concentric circle bins in the radial direction from the cylinder axis with radii equally spaced between *crmin* and *crmax*. For example, if *crmin* = 1.0 and *crmax* = 10.0 and *ncbin* = 9, then the first bin spans 1.0 < r < 2.0, and the last bin spans 9.0 < r 10.0. The geometry of the bins in the radial dimensions is the same whether the simulation box is orthogonal or triclinic; i.e. the concentric circles are not tilted or scaled differently in the two different dimensions to transform them into ellipses.

The created bins (and hence the chunk IDs) are numbered consecutively from 1 to the number of bins = *Nchunk*. For *bin2d* and *bin3d*, the numbering varies most rapidly in the first dimension (which could be x, y, or z), next rapidly in the 2nd dimension, and most slowly in the 3rd dimension. For *bin/sphere*, the bin with smallest radii is chunk 1 and the bni with largest radii is chunk Nchunk = *ncbin*. For *bin/cylinder*, the numbering varies most rapidly in the dimension along the cylinder axis and most slowly in the radial direction.

Each time this compute is invoked, each atom is mapped to a bin based on its current position. Note that between reneighboring timesteps, atoms can move outside the current simulation box. If the box is periodic (in that dimension) the atom is remapping into the periodic box for purposes of binning. If the box in not periodic, the atom may have moved outside the bounds of all bins. If an atom is not inside any bin, the *discard* keyword is used to determine how a chunk ID is assigned to the atom.

The *type* style uses the atom type as the chunk ID. *Nchunk* is set to the number of atom types defined for the simulation, e.g. via the *create_box* or *read_data* commands.

The *molecule* style uses the molecule ID of each atom as its chunk ID. *Nchunk* is set to the largest chunk ID. Note that this excludes molecule IDs for atoms which are not in the specified group or optional region.

There is no requirement that all atoms in a particular molecule are assigned the same chunk ID (zero or non-zero), though you probably want that to be the case, if you wish to compute a per-molecule property. LAMMPS will issue a warning if that is not the case, but only the first time that *Nchunk* is calculated.

Note that atoms with a molecule ID = 0, which may be non-molecular solvent atoms, have an out-of-range chunk ID. These atoms are discarded (not assigned to any chunk) or assigned to *Nchunk*, depending on the value of the *discard* keyword.

The *compute/fix/variable* styles set the chunk ID of each atom based on a quantity calculated and stored by a compute, fix, or variable. In each case, it must be a per-atom quantity. In each case the referenced floating point values are converted to an integer chunk ID as follows. The floating point value is truncated (rounded down) to an integer value. If the integer value is <= 0, then a chunk ID of 0 is assigned to the atom. If the integer value is > 0, it becomes the chunk ID to the atom. *Nchunk* is set to the largest chunk ID. Note that this excludes atoms which are not in the specified group or optional region.

If the style begins with "c_", a compute ID must follow which has been previously defined in the input script. If no bracketed integer is appended, the per-atom vector calculated by the compute is used. If a bracketed integer is appended, the Ith column of the per-atom array calculated by the compute is used. Users can also write code for their own compute styles and *add them to LAMMPS*.

If the style begins with "f_", a fix ID must follow which has been previously defined in the input script. If no bracketed integer is appended, the per-atom vector calculated by the fix is used. If a bracketed integer is appended, the Ith column of the per-atom array calculated by the fix is used. Note that some fixes only produce their values on certain timesteps, which must be compatible with the timestep on which this compute accesses the fix, else an error results. Users can also write code for their own fix styles and *add them to LAMMPS*.

If a value begins with "v_", a variable name for an *atom* or *atomfile* style *variable* must follow which has been previously defined in the input script. Variables of style *atom* can reference thermodynamic keywords and various

per-atom attributes, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of generating per-atom quantities to treat as a chunk ID.

Normally, *Nchunk* = the number of chunks, is re-calculated every time this fix is invoked, though the value may or may not change. As explained below, the *nchunk* keyword can be set to *once* which means *Nchunk* will never change.

If a *fix ave/chunk* command uses this compute, it can also turn off the re-calculation of *Nchunk* for one or more windows of timesteps. The extent of the windows, during which Nchunk is held constant, are determined by the *Nevery*, *Nrepeat*, *Nfreq* values and the *ave* keyword setting that are used by the *fix ave/chunk* command.

Specifically, if *ave* = *one*, then for each span of *Nfreq* timesteps, *Nchunk* is held constant between the first timestep when averaging is done (within the Nfreq-length window), and the last timestep when averaging is done (multiple of Nfreq). If *ave* = *running* or *window*, then *Nchunk* is held constant forever, starting on the first timestep when the *fix ave/chunk* command invokes this compute.

Note that multiple *fix ave/chunk* commands can use the same compute chunk/atom compute. However, the time windows they induce for holding *Nchunk* constant must be identical, else an error will be generated.

The various optional keywords operate as follows. Note that some of them function differently or are ignored by different chunk styles. Some of them also have different default values, depending on the chunk style, as listed below.

The *region* keyword applies to all chunk styles. If used, an atom must be in both the specified group and the specified geometric *region* to be assigned to a chunk.

The *nchunk* keyword applies to all chunk styles. It specifies how often *Nchunk* is recalculated, which in turn can affect the chunk IDs assigned to individual atoms.

If *nchunk* is set to *once*, then *Nchunk* is only calculated once, the first time this compute is invoked. If *nchunk* is set to *every*, then *Nchunk* is re-calculated every time the compute is invoked. Note that, as described above, the use of this compute by the *fix ave/chunk* command can override the *every* setting.

The default values for *nchunk* are listed below and depend on the chunk style and other system and keyword settings. They attempt to represent typical use cases for the various chunk styles. The *nchunk* value can always be set explicitly if desired.

The *limit* keyword can be used to limit the calculated value of *Nchunk* = the number of chunks. The limit is applied each time *Nchunk* is calculated, which also limits the chunk IDs assigned to any atom. The *limit* keyword is used by all chunk styles except the *binning* styles, which ignore it. This is because the number of bins can be tailored using the *bound* keyword (described below) which effectively limits the size of *Nchunk*.

If *limit* is set to *Nc* = 0, then no limit is imposed on *Nchunk*, though the *compress* keyword can still be used to reduce *Nchunk*, as described below.

If *Nc* > 0, then the effect of the *limit* keyword depends on whether the *compress* keyword is also used with a setting of *yes*, and whether the *compress* keyword is specified before the *limit* keyword or after.

In all cases, *Nchunk* is first calculated in the usual way for each chunk style, as described above.

First, here is what occurs if *compress yes* is not set. If *limit* is set to *Nc max*, then *Nchunk* is reset to the smaller of *Nchunk* and *Nc*. If *limit* is set to *Nc exact*, then *Nchunk* is reset to *Nc*, whether the original *Nchunk* was larger or smaller than *Nc*. If *Nchunk* shrank due to the *limit* setting, then atom chunk IDs > *Nchunk* will be reset to 0 or *Nchunk*, depending on the setting of the *discard* keyword. If *Nchunk* grew, there will simply be some chunks with no atoms assigned to them.

If *compress yes* is set, and the *compress* keyword comes before the *limit* keyword, the compression operation is performed first, as described below, which resets *Nchunk*. The *limit* keyword is then applied to the new *Nchunk* value, exactly as described in the preceding paragraph. Note that in this case, all atoms will end up with chunk IDs <= *Nc*, but their original values (e.g. molecule ID or compute/fix/variable) may have been > *Nc*, because of the compression operation.

If *compress yes* is set, and the *compress* keyword comes after the *limit* keyword, then the *limit* value of *Nc* is applied first to the uncompressed value of *Nchunk*, but only if *Nc* < *Nchunk* (whether *Nc max* or *Nc exact* is used). This effectively means all atoms with chunk IDs > *Nc* have their chunk IDs reset to 0 or *Nc*, depending on the setting of the *discard* keyword. The compression operation is then performed, which may shrink *Nchunk* further. If the new *Nchunk* < *Nc* and *limit* = *Nc exact* is specified, then *Nchunk* is reset to *Nc*, which results in extra chunks with no atoms assigned to them. Note that in this case, all atoms will end up with chunk IDs <= *Nc*, and their original values (e.g. molecule ID or compute/fix/variable value) will also have been <= *Nc*.

The *ids* keyword applies to all chunk styles. If the setting is *once* then the chunk IDs assigned to atoms the first time this compute is invoked will be permanent, and never be re-computed.

If the setting is *nfreq* and if a *fix ave/chunk* command is using this compute, then in each of the *Nchunk* = constant time windows (discussed above), the chunk ID's assigned to atoms on the first step of the time window will persist until the end of the time window.

If the setting is *every*, which is the default, then chunk IDs are re-calculated on any timestep this compute is invoked.

Note: If you want the persistent chunk-IDs calculated by this compute to be continuous when running from a *restart file*, then you should use the same ID for this compute, as in the original run. This is so that the fix this compute creates to store per-atom quantities will also have the same ID, and thus be initialized correctly with chunk IDs from the restart file.

The *compress* keyword applies to all chunk styles and affects how *Nchunk* is calculated, which in turn affects the chunk IDs assigned to each atom. It is useful for converting a "sparse" set of chunk IDs (with many IDs that have no atoms assigned to them), into a "dense" set of IDs, where every chunk has one or more atoms assigned to it.

Two possible use cases are as follows. If a large simulation box is mostly empty space, then the *binning* style may produce many bins with no atoms. If *compress* is set to *yes*, only bins with atoms will be contribute to *Nchunk*. Likewise, the *molecule* or *compute/fix/variable* styles may produce large *Nchunk* values. For example, the *compute cluster/atom* command assigns every atom an atom ID for one of the atoms it is clustered with. For a million-atom system with 5 clusters, there would only be 5 unique chunk IDs, but the largest chunk ID might be 1 million, resulting in *Nchunk* = 1 million. If *compress* is set to *yes*, *Nchunk* will be reset to 5.

If *compress* is set to *no*, which is the default, no compression is done. If it is set to *yes*, all chunk IDs with no atoms are removed from the list of chunk IDs, and the list is sorted. The remaining chunk IDs are renumbered from 1 to *Nchunk* where *Nchunk* is the new length of the list. The chunk IDs assigned to each atom reflect the new renumbering from 1 to *Nchunk*.

The original chunk IDs (before renumbering) can be accessed by the *compute property/chunk* command and its *id* keyword, or by the *fix ave/chunk* command which outputs the original IDs as one of the columns in its global output array. For example, using the "compute cluster/atom" command discussed above, the original 5 unique chunk IDs might be atom IDs (27,4982,58374,857838,1000000). After compression, these will be renumbered to (1,2,3,4,5). The original values (27,. . . ,1000000) can be output to a file by the *fix ave/chunk* command, or by using the *fix ave/time* command in conjunction with the *compute property/chunk* command.

Note: The compression operation requires global communication across all processors to share their chunk ID values. It can require large memory on every processor to store them, even after they are compressed, if there are a

large number of unique chunk IDs with atoms assigned to them. It uses a STL map to find unique chunk IDs and store them in sorted order. Each time an atom is assigned a compressed chunk ID, it must access the STL map. All of this means that compression can be expensive, both in memory and CPU time. The use of the *limit* keyword in conjunction with the *compress* keyword can affect these costs, depending on which keyword is used first. So use this option with care.

The *discard* keyword applies to all chunk styles. It affects what chunk IDs are assigned to atoms that do not match one of the valid chunk IDs from 1 to *Nchunk*. Note that it does not apply to atoms that are not in the specified group or optionally specified region. Those atoms are always assigned a chunk ID = 0.

If the calculated chunk ID for an atom is not within the range 1 to *Nchunk* then it is a "discard" atom. Note that *Nchunk* may have been shrunk by the *limit* keyword. Or the *compress* keyword may have eliminated chunk IDs that were valid before the compression took place, and are now not in the compressed list. Also note that for the *molecule* chunk style, if new molecules are added to the system, their chunk IDs may exceed a previously calculated *Nchunk*. Likewise, evaluation of a compute/fix/variable on a later timestep may return chunk IDs that are invalid for the previously calculated *Nchunk*.

All the chunk styles except the *binning* styles, must use *discard* set to either *yes* or *no*. If *discard* is set to *yes*, which is the default, then every "discard" atom has its chunk ID set to 0. If *discard* is set to *no*, every "discard" atom has its chunk ID set to *Nchunk*. I.e. it becomes part of the last chunk.

The *binning* styles use the *discard* keyword to decide whether to discard atoms outside the spatial domain covered by bins, or to assign them to the bin they are nearest to.

For the *bin/1d*, *bin/2d*, *bin/3d* styles the details are as follows. If *discard* is set to *yes*, an out-of-domain atom will have its chunk ID set to 0. If *discard* is set to *no*, the atom will have its chunk ID set to the first or last bin in that dimension. If *discard* is set to *mixed*, which is the default, it will only have its chunk ID set to the first or last bin if bins extend to the simulation box boundary in that dimension. This is the case if the *bound* keyword settings are *lower* and *upper*, which is the default. If the *bound* keyword settings are numeric values, then the atom will have its chunk ID set to 0 if it is outside the bounds of any bin. Note that in this case, it is possible that the first or last bin extends beyond the numeric *bounds* settings, depending on the specified *origin*. If this is the case, the chunk ID of the atom is only set to 0 if it is outside the first or last bin, not if it is simply outside the numeric *bounds* setting.

For the *bin/sphere* style the details are as follows. If *discard* is set to *yes*, an out-of-domain atom will have its chunk ID set to 0. If *discard* is set to *no* or *mixed*, the atom will have its chunk ID set to the first or last bin, i.e. the innermost or outermost spherical shell. If the distance of the atom from the origin is less than *rmin*, it will be assigned to the first bin. If the distance of the atom from the origin is greater than *rmax*, it will be assigned to the last bin.

For the *bin/cylinder* style the details are as follows. If *discard* is set to *yes*, an out-of-domain atom will have its chunk ID set to 0. If *discard* is set to *no*, the atom will have its chunk ID set to the first or last bin in both the radial and axis dimensions. If *discard* is set to *mixed*, which is the default, the radial dimension is treated the same as for *discard* = no. But for the axis dimension, it will only have its chunk ID set to the first or last bin if bins extend to the simulation box boundary in the axis dimension. This is the case if the *bound* keyword settings are *lower* and *upper*, which is the default. If the *bound* keyword settings are numeric values, then the atom will have its chunk ID set to 0 if it is outside the bounds of any bin. Note that in this case, it is possible that the first or last bin extends beyond the numeric *bounds* settings, depending on the specified *origin*. If this is the case, the chunk ID of the atom is only set to 0 if it is outside the first or last bin, not if it is simply outside the numeric *bounds* setting.

If *discard* is set to *no* or *mixed*, the atom will have its chunk ID set to the first or last bin, i.e. the innermost or outermost spherical shell. If the distance of the atom from the origin is less than *rmin*, it will be assigned to the first bin. If the distance of the atom from the origin is greater than *rmax*, it will be assigned to the last bin.

The *bound* keyword only applies to the *bin/1d*, *bin/2d*, *bin/3d* styles and to the axis dimension of the *bin/cylinder* style; otherwise it is ignored. It can be used one or more times to limit the extent of bin coverage in a specified dimension,

i.e. to only bin a portion of the box. If the *lo* setting is *lower* or the *hi* setting is *upper*, the bin extent in that direction extends to the box boundary. If a numeric value is used for *lo* and/or *hi*, then the bin extent in the *lo* or *hi* direction extends only to that value, which is assumed to be inside (or at least near) the simulation box boundaries, though LAMMPS does not check for this. Note that using the *bound* keyword typically reduces the total number of bins and thus the number of chunks *Nchunk*.

The *pbc* keyword only applies to the *bin/sphere* and *bin/cylinder* styles. If set to *yes*, the distance an atom is from the sphere origin or cylinder axis is calculated in a minimum image sense with respect to periodic dimensions, when determining which bin the atom is in. I.e. if x is a periodic dimension and the distance between the atom and the sphere center in the x dimension is greater than 0.5 * simulation box length in x, then a box length is subtracted to give a distance < 0.5 * simulation box length. This allosws the sphere or cylinder center to be near a box edge, and atoms on the other side of the periodic box will still be close to the center point/axis. Note that with a setting of *yes*, the outer sphere or cylinder radius must also be <= 0.5 * simulation box length in any periodic dimension except for the cylinder axis dimension, or an error is generated.

The *units* keyword only applies to the *binning* styles; otherwise it is ignored. For the *bin/1d*, *bin/2d*, *bin/3d* styles, it determines the meaning of the distance units used for the bin sizes *delta* and for *origin* and *bounds* values if they are coordinate values. For the *bin/sphere* style it determines the meaning of the distance units used for *xorig*,*yorig*,*zorig* and the radii *srmin* and *srmax*. For the *bin/cylinder* style it determines the meaning of the distance units used for *delta*,*c1*,*c2* and the radii *crmin* and *crmax*.

For orthogonal simulation boxes, any of the 3 options may be used. For non-orthogonal (triclinic) simulation boxes, only the *reduced* option may be used.

A *box* value selects standard distance units as defined by the *units* command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacing. A *reduced* value means normalized unitless values between 0 and 1, which represent the lower and upper faces of the simulation box respectively. Thus an *origin* value of 0.5 means the center of the box in any dimension. A *delta* value of 0.1 means 10 bins span the box in that dimension.

Note that for the *bin/sphere* style, the radii *srmin* and *srmax* are scaled by the lattice spacing or reduced value of the *x* dimension.

Note that for the *bin/cylinder* style, the radii *crmin* and *crmax* are scaled by the lattice spacing or reduced value of the 1st dimension perpendicular to the cylinder axis. E.g. y for an x-axis cylinder, x for a y-axis cylinder, and x for a z-axis cylinder.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values are unitless chunk IDs, ranging from 1 to *Nchunk* (inclusive) for atoms assigned to chunks, and 0 for atoms not belonging to a chunk.

17.11.4 Restrictions

Even if the *nchunk* keyword is set to *once*, the chunk IDs assigned to each atom are not stored in a restart files. This means you cannot expect those assignments to persist in a restarted simulation. Instead you must re-specify this command and assign atoms to chunks when the restarted simulation begins.

17.11.5 Related commands

fix ave/chunk, *compute global/atom*

17.11.6 Default

The option defaults are as follows:

- region = none
- nchunk = every, if compress is yes, overriding other defaults listed here
- nchunk = once, for type style
- nchunk = once, for mol style if region is none
- nchunk = every, for mol style if region is set
- nchunk = once, for binning style if the simulation box size is static or units = reduced
- nchunk = every, for binning style if the simulation box size is dynamic and units is lattice or box
- nchunk = every, for compute/fix/variable style
- limit = 0
- ids = every
- compress = no
- discard = yes, for all styles except binning
- discard = mixed, for binning styles
- bound = lower and upper in all dimensions
- pbc = no
- units = lattice

17.12 compute chunk/spread/atom command

17.12.1 Syntax

```
compute ID group-ID chunk/spread/atom chunkID input1 input2 ...
```

- ID, group-ID are documented in *compute* command
- chunk/spread/atom = style name of this compute command
- chunkID = ID of *compute chunk/atom* command
- one or more inputs can be listed
- input = c_ID, c_ID[N], f_ID, f_ID[N]

```
c_ID = global vector calculated by a compute with ID
c_ID[I] = Ith column of global array calculated by a compute with ID, I can␣
↪include wildcard (see below)
f_ID = global vector calculated by a fix with ID
f_ID[I] = Ith column of global array calculated by a fix with ID, I can include␣
↪wildcard (see below)
```

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17.12.2 Examples

```
compute 1 all chunk/spread/atom mychunk c_com[*] c_gyration
```

17.12.3 Description

Define a calculation that "spreads" one or more per-chunk values to each atom in the chunk. This can be useful in several scenarios:

- For creating a *dump file* where each atom lists info about the chunk it is in, e.g. for post-processing purposes.
- To access chunk value in *atom-style variables* that need info about the chunk each atom is in.
- To use the *fix ave/chunk* command to spatially average per-chunk values calculated by a per-chunk compute.

Examples are given below.

In LAMMPS, chunks are collections of atoms defined by a *compute chunk/atom* command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the *compute chunk/atom* and *Howto chunk* doc pages for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

For inputs that are computes, they must be a compute that calculates per-chunk values. These are computes whose style names end in "/chunk".

For inputs that are fixes, they should be a fix that calculates per-chunk values. For example, *fix ave/chunk* or *fix ave/time* (assuming it is time-averaging per-chunk data).

For each atom, this compute accesses its chunk ID from the specified *chunkID* compute, then accesses the per-chunk value in each input. Those values are copied to this compute to become the output for that atom.

The values generated by this compute will be 0.0 for atoms not in the specified compute group *group-ID*. They will also be 0.0 if the atom is not in a chunk, as assigned by the *chunkID* compute. They will also be 0.0 if the current chunk ID for the atom is out-of-bounds with respect to the number of chunks stored by a particular input compute or fix.

Note: LAMMPS does not check that a compute or fix which calculates per-chunk values uses the same definition of chunks as this compute. It's up to you to be consistent. Likewise, for a fix input, LAMMPS does not check that it is per-chunk data. It only checks that the fix produces a global vector or array.

Each listed input is operated on independently.

If a bracketed index I is used, it can be specified using a wildcard asterisk with the index to effectively specify multiple values. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of columns in the array, then an asterisk with no numeric values means all indices from 1 to N. A leading asterisk means all indices from 1 to n (inclusive). A trailing asterisk means all indices from n to N (inclusive). A middle asterisk means all indices from m to n (inclusive).

Using a wildcard is the same as if the individual columns of the array had been listed one by one. E.g. these 2 compute chunk/spread/atom commands are equivalent, since the *compute com/chunk* command creates a per-atom array with 3 columns:

```
compute com all com/chunk mychunk
compute 10 all chunk/spread/atom mychunk c_com[*]
compute 10 all chunk/spread/atom mychunk c_com[1] c_com[2] c_com[3]
```

Here is an example of writing a dump file the with the center-of-mass (COM) for the chunk each atom is in. The commands below can be added to the bench/in.chain script.

```
compute         cmol all chunk/atom molecule
compute         com all com/chunk cmol
compute         comchunk all chunk/spread/atom cmol c_com[*]
dump            1 all custom 50 tmp.dump id mol type x y z c_comchunk[*]
dump_modify     1 sort id
```

The same per-chunk data for each atom could be used to define per-atom forces for the *fix addforce* command. In this example the forces act to pull atoms of an extended polymer chain towards its COM in an attractive manner.

```
compute         prop all property/atom xu yu zu
variable        k equal 0.1
variable        fx atom v_k*(c_comchunk[1]-c_prop[1])
variable        fy atom v_k*(c_comchunk[2]-c_prop[2])
variable        fz atom v_k*(c_comchunk[3]-c_prop[3])
fix             3 all addforce v_fx v_fy v_fz
```

Note that *compute property/atom* is used to generate unwrapped coordinates for use in the per-atom force calculation, so that the effect of periodic boundaries is accounted for properly.

Over time this applied force could shrink each polymer chain's radius of gyration in a polymer mixture simulation. Here is output from the bench/in.chain script. Thermo output is shown for 1000 steps, where the last column is the average radius of gyration over all 320 chains in the 32000 atom system:

```
compute         gyr all gyration/chunk cmol
variable        ave equal ave(c_gyr)
thermo_style    custom step etotal press v_ave

       0    22.394765    4.6721833     5.128278
     100    22.445002    4.8166709    5.0348372
     200    22.500128    4.8790392    4.9364875
     300    22.534686    4.9183766    4.8590693
     400    22.557196    4.9492211    4.7937849
     500    22.571017    4.9161853    4.7412008
     600    22.573944    5.0229708    4.6931243
     700    22.581804    5.0541301    4.6440647
     800    22.584683    4.9691734    4.6000016
     900     22.59128    5.0247538    4.5611513
    1000    22.586832      4.94697    4.5238362
```

Here is an example for using one set of chunks, defined for molecules, to compute the dipole moment vector for each chunk. E.g. for water molecules. Then spreading those values to each atom in each chunk. Then defining a second set of chunks based on spatial bins. And finally, using the *fix ave/chunk* command to calculate an average dipole moment vector per spatial bin.

```
compute       cmol all chunk/atom molecule
compute       dipole all dipole/chunk cmol
compute       spread all chunk/spread/atom cmol c_dipole[1] c_dipole[2] c_
↪dipole[3]
```

```
compute       cspatial all chunk/atom bin/1d z lower 0.1 units reduced
fix           ave all ave/chunk 100 10 1000 cspatial c_spread[*]
```

Note that the *fix ave/chunk* command requires per-atom values as input. That is why the compute chunk/spread/atom command is used to assign per-chunk values to each atom in the chunk. If a molecule straddles bin boundaries, each of its atoms contributes in a weighted manner to the average dipole moment of the spatial bin it is in.

Output info:

This compute calculates a per-atom vector or array, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The output is a per-atom vector if a single input value is specified, otherwise a per-atom array is output. The number of columns in the array is the number of inputs provided. The per-atom values for the vector or each column of the array will be in whatever *units* the corresponding input value is in.

The vector or array values are "intensive".

17.12.4 Restrictions

none

17.12.5 Related commands

compute chunk/atom, *fix ave/chunk*, *compute reduce/chunk*

Default: none

17.13 compute cluster/atom command

17.14 compute fragment/atom command

17.15 compute aggregate/atom command

17.15.1 Syntax

```
compute ID group-ID cluster/atom cutoff
compute ID group-ID fragment/atom
compute ID group-ID aggregate/atom cutoff
```

- ID, group-ID are documented in *compute* command
- *cluster/atom* or *fragment/atom* or *aggregate/atom* = style name of this compute command
- cutoff = distance within which to label atoms as part of same cluster (distance units)

17.15.2 Examples

```
compute 1 all cluster/atom 3.5
compute 1 all fragment/atom

compute 1 all aggregate/atom 3.5
```

17.15.3 Description

Define a computation that assigns each atom a cluster, fragment, or aggregate ID.

A cluster is defined as a set of atoms, each of which is within the cutoff distance from one or more other atoms in the cluster. If an atom has no neighbors within the cutoff distance, then it is a 1-atom cluster.

A fragment is similarly defined as a set of atoms, each of which has an explicit bond (i.e. defined via a *data file*, the *create_bonds* command, or through fixes like *fix bond/create*, *fix bond/swap*, or *fix bond/break*). The cluster ID or fragment ID of every atom in the cluster will be set to the smallest atom ID of any atom in the cluster or fragment, respectively.

An aggregate is defined by combining the rules for clusters and fragments, i.e. a set of atoms, where each of it is within the cutoff distance from one or more atoms within a fragment that is part of the same cluster. This measure can be used to track molecular assemblies like micelles.

Only atoms in the compute group are clustered and assigned cluster IDs. Atoms not in the compute group are assigned a cluster ID = 0. For fragments, only bonds where **both** atoms of the bond are included in the compute group are assigned to fragments, so that only fragments are detected where **all** atoms are in the compute group. Thus atoms may be included in the compute group, yes still have a fragment ID of 0.

For computes *cluster/atom* and *aggregate/atom* the neighbor list needed to compute this quantity is constructed each time the calculation is performed (i.e. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently or to have multiple compute/dump commands, each of a *cluster/atom* or *aggregate/atom* style.

Note: If you have a bonded system, then the settings of *special_bonds* command can remove pairwise interactions between atoms in the same bond, angle, or dihedral. This is the default setting for the *special_bonds* command, and means those pairwise interactions do not appear in the neighbor list. Because this fix uses the neighbor list, it also means those pairs will not be included when computing the clusters. This does not apply when using long-range coulomb (*coul/long*, *coul/msm*, *coul/wolf* or similar. One way to get around this would be to set special_bond scaling factors to very tiny numbers that are not exactly zero (e.g. 1.0e-50). Another workaround is to write a dump file, and use the *rerun* command to compute the clusters for snapshots in the dump file. The rerun script can use a *special_bonds* command that includes all pairs in the neighbor list.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values will be an ID > 0, as explained above.

17.15.4 Restrictions

none

17.15.5 Related commands

compute coord/atom

Default: none

17.16 compute cna/atom command

17.16.1 Syntax

```
compute ID group-ID cna/atom cutoff
```

- ID, group-ID are documented in *compute* command
- cna/atom = style name of this compute command
- cutoff = cutoff distance for nearest neighbors (distance units)

17.16.2 Examples

```
compute 1 all cna/atom 3.08
```

17.16.3 Description

Define a computation that calculates the CNA (Common Neighbor Analysis) pattern for each atom in the group. In solid-state systems the CNA pattern is a useful measure of the local crystal structure around an atom. The CNA methodology is described in *(Faken)* and *(Tsuzuki)*.

Currently, there are five kinds of CNA patterns LAMMPS recognizes:

- fcc = 1
- hcp = 2
- bcc = 3
- icosahedral = 4
- unknown = 5

The value of the CNA pattern will be 0 for atoms not in the specified compute group. Note that normally a CNA calculation should only be performed on mono-component systems.

The CNA calculation can be sensitive to the specified cutoff value. You should insure the appropriate nearest neighbors of an atom are found within the cutoff distance for the presumed crystal structure. E.g. 12 nearest neighbor for perfect

FCC and HCP crystals, 14 nearest neighbors for perfect BCC crystals. These formulas can be used to obtain a good cutoff distance:

$$r_c^{fcc} = \frac{1}{2}\left(\frac{\sqrt{2}}{2}+1\right)\text{a} \simeq 0.8536\text{ a}$$
$$r_c^{bcc} = \frac{1}{2}(\sqrt{2}+1)\text{a} \simeq 1.207\text{ a}$$
$$r_c^{hcp} = \frac{1}{2}\left(1+\sqrt{\frac{4+2x^2}{3}}\right)\text{a}$$

where a is the lattice constant for the crystal structure concerned and in the HCP case, x = (c/a) / 1.633, where 1.633 is the ideal c/a for HCP crystals.

Also note that since the CNA calculation in LAMMPS uses the neighbors of an owned atom to find the nearest neighbors of a ghost atom, the following relation should also be satisfied:

$$r_c + r_s > 2 * \text{cutoff}$$

where r_c is the cutoff distance of the potential, r_s is the skin distance as specified by the *neighbor* command, and cutoff is the argument used with the compute cna/atom command. LAMMPS will issue a warning if this is not the case.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (e.g. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently or to have multiple compute/dump commands, each with a *cna/atom* style.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values will be a number from 0 to 5, as explained above.

17.16.4 Restrictions

none

17.16.5 Related commands

compute centro/atom

Default: none

(Faken) Faken, Jonsson, Comput Mater Sci, 2, 279 (1994).

(Tsuzuki) Tsuzuki, Branicio, Rino, Comput Phys Comm, 177, 518 (2007).

17.17 compute cnp/atom command

17.17.1 Syntax

```
compute ID group-ID cnp/atom cutoff
```

- ID, group-ID are documented in *compute* command
- cnp/atom = style name of this compute command
- cutoff = cutoff distance for nearest neighbors (distance units)

17.17.2 Examples

```
compute 1 all cnp/atom 3.08
```

17.17.3 Description

Define a computation that calculates the Common Neighborhood Parameter (CNP) for each atom in the group. In solid-state systems the CNP is a useful measure of the local crystal structure around an atom and can be used to characterize whether the atom is part of a perfect lattice, a local defect (e.g. a dislocation or stacking fault), or at a surface.

The value of the CNP parameter will be 0.0 for atoms not in the specified compute group. Note that normally a CNP calculation should only be performed on single component systems.

This parameter is computed using the following formula from *(Tsuzuki)*

$$Q_i = \frac{1}{n_i} \sum_{j=1}^{n_i} |\sum_{k=1}^{n_{ij}} \vec{R}_{ik} + \vec{R}_{jk}|^2$$

where the index *j* goes over the n_i nearest neighbors of atom *i*, and the index *k* goes over the n_{ij} common nearest neighbors between atom *i* and atom *j*. $\vec{R}_{ik}$ and $\vec{R}_{jk}$ are the vectors connecting atom *k* to atoms *i* and *j*. The quantity in the double sum is computed for each atom.

The CNP calculation is sensitive to the specified cutoff value. You should ensure that the appropriate nearest neighbors of an atom are found within the cutoff distance for the presumed crystal structure. E.g. 12 nearest neighbor for perfect FCC and HCP crystals, 14 nearest neighbors for perfect BCC crystals. These formulas can be used to obtain a good cutoff distance:

$$\begin{aligned} r_c^{fcc} =& \frac{1}{2}\left(\frac{\sqrt{2}}{2}+1\right) \mathrm{a} \simeq 0.8536\ \mathrm{a} \\ r_c^{bcc} =& \frac{1}{2}(\sqrt{2}+1)\mathrm{a} \simeq 1.207\ \mathrm{a} \\ r_c^{hcp} =& \frac{1}{2}\left(1+\sqrt{\frac{4+2x^2}{3}}\right) \mathrm{a} \end{aligned}$$

where a is the lattice constant for the crystal structure concerned and in the HCP case, x = (c/a) / 1.633, where 1.633 is the ideal c/a for HCP crystals.

Also note that since the CNP calculation in LAMMPS uses the neighbors of an owned atom to find the nearest neighbors of a ghost atom, the following relation should also be satisfied:

$$r_c + r_s > 2 * \mathrm{cutoff}$$

where r_c is the cutoff distance of the potential, r_s is the skin distance as specified by the *neighbor* command, and cutoff is the argument used with the compute cnp/atom command. LAMMPS will issue a warning if this is not the case.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (e.g. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently or to have multiple compute/dump commands, each with a *cnp/atom* style.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values will be real positive numbers. Some typical CNP values:

```
FCC lattice = 0.0
BCC lattice = 0.0
HCP lattice = 4.4

FCC (111) surface ~ 13.0
FCC (100) surface ~ 26.5
FCC dislocation core ~ 11
```

17.17.4 Restrictions

This compute is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.17.5 Related commands

compute cna/atom compute centro/atom

Default: none

(Tsuzuki) Tsuzuki, Branicio, Rino, Comput Phys Comm, 177, 518 (2007).

17.18 compute com command

17.18.1 Syntax

```
compute ID group-ID com
```

- ID, group-ID are documented in *compute* command
- com = style name of this compute command

17.18.2 Examples

```
compute 1 all com
```

17.18.3 Description

Define a computation that calculates the center-of-mass of the group of atoms, including all effects due to atoms passing through periodic boundaries.

A vector of three quantities is calculated by this compute, which are the x,y,z coordinates of the center of mass.

Note: The coordinates of an atom contribute to the center-of-mass in "unwrapped" form, by using the image flags associated with each atom. See the *dump custom* command for a discussion of "unwrapped" coordinates. See the Atoms section of the *read_data* command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the *set image* command.

Output info:

This compute calculates a global vector of length 3, which can be accessed by indices 1-3 by any command that uses global vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector values are "intensive". The vector values will be in distance *units*.

17.18.4 Restrictions

none

17.18.5 Related commands

compute com/chunk

Default: none

17.19 compute com/chunk command

17.19.1 Syntax

```
compute ID group-ID com/chunk chunkID
```

- ID, group-ID are documented in *compute* command
- com/chunk = style name of this compute command
- chunkID = ID of *compute chunk/atom* command

17.19.2 Examples

```
compute 1 fluid com/chunk molchunk
```

17.19.3 Description

Define a computation that calculates the center-of-mass for multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a *compute chunk/atom* command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the *compute chunk/atom* and *Howto chunk* doc pages for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

This compute calculates the x,y,z coordinates of the center-of-mass for each chunk, which includes all effects due to atoms passing through periodic boundaries.

Note that only atoms in the specified group contribute to the calculation. The *compute chunk/atom* command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

Note: The coordinates of an atom contribute to the chunk's center-of-mass in "unwrapped" form, by using the image flags associated with each atom. See the *dump custom* command for a discussion of "unwrapped" coordinates. See the Atoms section of the *read_data* command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the *set image* command.

The simplest way to output the results of the compute com/chunk calculation to a file is to use the *fix ave/time* command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all com/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk[*] file tmp.out mode vector
```

Output info:

This compute calculates a global array where the number of rows = the number of chunks *Nchunk* as calculated by the specified *compute chunk/atom* command. The number of columns = 3 for the x,y,z center-of-mass coordinates of each chunk. These values can be accessed by any command that uses global array values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The array values are "intensive". The array values will be in distance *units*.

17.19.4 Restrictions

none

17.19.5 Related commands

compute com

Default: none

17.20 compute contact/atom command

17.20.1 Syntax

```
compute ID group-ID contact/atom
```

- ID, group-ID are documented in *compute* command
- contact/atom = style name of this compute command

17.20.2 Examples

```
compute 1 all contact/atom
```

17.20.3 Description

Define a computation that calculates the number of contacts for each atom in a group.

The contact number is defined for finite-size spherical particles as the number of neighbor atoms which overlap the central particle, meaning that their distance of separation is less than or equal to the sum of the radii of the two particles.

The value of the contact number will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, whose values can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values will be a number >= 0.0, as explained above.

17.20.4 Restrictions

This compute requires that atoms store a radius as defined by the *atom_style sphere* command.

17.20.5 Related commands

compute coord/atom

Default: none

17.21 compute coord/atom command

17.21.1 Syntax

```
compute ID group-ID coord/atom cstyle args ...
```

- ID, group-ID are documented in *compute* command
- coord/atom = style name of this compute command
- cstyle = *cutoff* or *orientorder*

```
cutoff args = cutoff [group group2-ID] typeN
  cutoff = distance within which to count coordination neighbors␣
↪(distance units)
  group group2-ID = select group-ID to restrict which atoms to consider␣
↪for coordination number (optional)
  typeN = atom type for Nth coordination count (see asterisk form below)
orientorder args = orientorderID threshold
  orientorderID = ID of an orientorder/atom compute
  threshold = minimum value of the product of two "connected" atoms
```

17.21.2 Examples

```
compute 1 all coord/atom cutoff 2.0
compute 1 all coord/atom cutoff 6.0 1 2
compute 1 all coord/atom cutoff 6.0 2*4 5*8 *
compute 1 solute coord/atom cutoff 2.0 group solvent
compute 1 all coord/atom orientorder 2 0.5
```

17.21.3 Description

This compute performs calculations between neighboring atoms to determine a coordination value. The specific calculation and the meaning of the resulting value depend on the *cstyle* keyword used.

The *cutoff* cstyle calculates one or more traditional coordination numbers for each atom. A coordination number is defined as the number of neighbor atoms with specified atom type(s), and optionally within the specified group, that are within the specified cutoff distance from the central atom. The compute group selects only the central atoms; all neighboring atoms, unless selected by type, type range, or group option, are included in the coordination number tally.

The optional *group* keyword allows to specify from which group atoms contribute to the coordination number. Default setting is group 'all'.

The *typeN* keywords allow specification of which atom types contribute to each coordination number. One coordination number is computed for each of the *typeN* keywords listed. If no *typeN* keywords are listed, a single coordination number is calculated, which includes atoms of all types (same as the "*" format, see below).

The *typeN* keywords can be specified in one of two ways. An explicit numeric value can be used, as in the 2nd example above. Or a wild-card asterisk can be used to specify a range of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

The *orientorder* cstyle calculates the number of "connected" neighbor atoms J around each central atom I. For this *cstyle*, connected is defined by the orientational order parameter calculated by the *compute orientorder/atom* command.

This *cstyle* thus allows one to apply the ten Wolde's criterion to identify crystal-like atoms in a system, as discussed in *ten Wolde*.

The ID of the previously specified *compute orientorder/atom* command is specified as *orientorderID*. The compute must invoke its *components* option to calculate components of the *Ybar_lm* vector for each atoms, as described in its documentation. Note that orientorder/atom compute defines its own criteria for identifying neighboring atoms. If the scalar product (*Ybar_lm(i)*,*Ybar_lm(j)*), calculated by the orientorder/atom compute is larger than the specified *threshold*, then I and J are connected, and the coordination value of I is incremented by one.

For all *cstyle* settings, all coordination values will be 0.0 for atoms not in the specified compute group.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (i.e. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently.

Note: If you have a bonded system, then the settings of *special_bonds* command can remove pairwise interactions between atoms in the same bond, angle, or dihedral. This is the default setting for the *special_bonds* command, and means those pairwise interactions do not appear in the neighbor list. Because this fix uses the neighbor list, it also means those pairs will not be included in the coordination count. One way to get around this, is to write a dump file, and use the *rerun* command to compute the coordination for snapshots in the dump file. The rerun script can use a *special_bonds* command that includes all pairs in the neighbor list.

Output info:

For *cstyle* cutoff, this compute can calculate a per-atom vector or array. If single *type1* keyword is specified (or if none are specified), this compute calculates a per-atom vector. If multiple *typeN* keywords are specified, this compute calculates a per-atom array, with N columns.

For *cstyle* orientorder, this compute calculates a per-atom vector.

These values can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector or array values will be a number >= 0.0, as explained above.

17.21.4 Restrictions

none

17.21.5 Related commands

compute cluster/atom compute orientorder/atom

17.21.6 Default

group = all

(tenWolde) P. R. ten Wolde, M. J. Ruiz-Montero, D. Frenkel, J. Chem. Phys. 104, 9932 (1996).

17.22 compute damage/atom command

17.22.1 Syntax

```
compute ID group-ID damage/atom
```

- ID, group-ID are documented in *compute* command
- damage/atom = style name of this compute command

17.22.2 Examples

```
compute 1 all damage/atom
```

17.22.3 Description

Define a computation that calculates the per-atom damage for each atom in a group. This is a quantity relevant for *Peridynamics models*. See this document for an overview of LAMMPS commands for Peridynamics modeling.

The "damage" of a Peridynamics particles is based on the bond breakage between the particle and its neighbors. If all the bonds are broken the particle is considered to be fully damaged.

See the PDLAMMPS user guide for a formal definition of "damage" and more details about Peridynamics as it is implemented in LAMMPS.

This command can be used with all the Peridynamic pair styles.

The damage value will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values are unitless numbers (damage) >= 0.0.

17.22.4 Restrictions

This compute is part of the PERI package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.22.5 Related commands

compute dilatation/atom, *compute plasticity/atom*

Default: none

17.23 compute dihedral command

17.23.1 Syntax

```
compute ID group-ID dihedral
```

- ID, group-ID are documented in *compute* command
- dihedral = style name of this compute command

17.23.2 Examples

```
compute 1 all dihedral
```

17.23.3 Description

Define a computation that extracts the dihedral energy calculated by each of the dihedral sub-styles used in the *dihedral_style hybrid* command. These values are made accessible for output or further processing by other commands. The group specified for this command is ignored.

This compute is useful when using *dihedral_style hybrid* if you want to know the portion of the total energy contributed by one or more of the hybrid sub-styles.

Output info:

This compute calculates a global vector of length N where N is the number of sub_styles defined by the *dihedral_style hybrid* command. which can be accessed by indices 1-N. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector values are "extensive" and will be in energy *units*.

17.23.4 Restrictions

none

17.23.5 Related commands

compute pe, *compute pair*

Default: none

17.24 compute dihedral/local command

17.24.1 Syntax

```
compute ID group-ID dihedral/local value1 value2 ... keyword args ...
```

- ID, group-ID are documented in *compute* command
- dihedral/local = style name of this compute command
- one or more values may be appended
- value = *phi* or *v_name*

  ```
  phi = tabulate dihedral angles
  v_name = equal-style variable with name (see below)
  ```

- zero or more keyword/args pairs may be appended
- keyword = *set*

  ```
  set args = phi name
    phi = only currently allowed arg
    name = name of variable to set with phi
  ```

17.24.2 Examples

```
compute 1 all dihedral/local phi

compute 1 all dihedral/local phi v_cos set phi p
```

17.24.3 Description

Define a computation that calculates properties of individual dihedral interactions. The number of datums generated, aggregated across all processors, equals the number of dihedral angles in the system, modified by the group parameter as explained below.

The value *phi* is the dihedral angle, as defined in the diagram on the *dihedral_style* doc page.

The value *v_name* can be used together with the *set* keyword to compute a user-specified function of the dihedral angle phi. The *name* specified for the *v_name* value is the name of an *equal-style variable* which should evaluate a formula based on a variable which will store the angle phi. This other variable must be an *internal-style variable* defined in the input script; its initial numeric value can be anything. It must be an internal-style variable, because this command resets its value directly. The *set* keyword is used to identify the name of this other variable associated with phi.

Note that the value of phi for each angle which stored in the internal variable is in radians, not degrees.

As an example, these commands can be added to the bench/in.rhodo script to compute the cosine and cosine^2 of every dihedral angle in the system and output the statistics in various ways:

```
variable p internal 0.0
variable cos equal cos(v_p)
variable cossq equal cos(v_p)*cos(v_p)

compute 1 all property/local datom1 datom2 datom3 datom4 dtype
compute 2 all dihedral/local phi v_cos v_cossq set phi p
```

```
dump 1 all local 100 tmp.dump c_1[*] c_2[*]

compute 3 all reduce ave c_2[*]
thermo_style custom step temp press c_3[*]

fix 10 all ave/histo 10 10 100 -1 1 20 c_2[2] mode vector file tmp.histo
```

The *dump local* command will output the angle, cosine(angle), cosine^2(angle) for every dihedral in the system. The *thermo_style* command will print the average of those quantities via the *compute reduce* command with thermo output. And the *fix ave/histo* command will histogram the cosine(angle) values and write them to a file.

The local data stored by this command is generated by looping over all the atoms owned on a processor and their dihedrals. A dihedral will only be included if all 4 atoms in the dihedral are in the specified compute group.

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For example, dihedral output from the *compute property/local* command can be combined with data from this command and output by the *dump local* command in a consistent way.

Here is an example of how to do this:

```
compute 1 all property/local dtype datom1 datom2 datom3 datom4
compute 2 all dihedral/local phi
dump 1 all local 1000 tmp.dump index c_1[1] c_1[2] c_1[3] c_1[4] c_1[5] c_2[1]
```

Output info:

This compute calculates a local vector or local array depending on the number of values. The length of the vector or number of rows in the array is the number of dihedrals. If a single value is specified, a local vector is produced. If two or more values are specified, a local array is produced where the number of columns = the number of values. The vector or array can be accessed by any command that uses local values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The output for *phi* will be in degrees.

17.24.4 Restrictions

none

17.24.5 Related commands

dump local, *compute property/local*

Default: none

17.25 compute dilatation/atom command

17.25.1 Syntax

```
compute ID group-ID dilatation/atom
```

- ID, group-ID are documented in compute command
- dilation/atom = style name of this compute command

17.25.2 Examples

```
compute 1 all dilatation/atom
```

17.25.3 Description

Define a computation that calculates the per-atom dilatation for each atom in a group. This is a quantity relevant for *Peridynamics models*. See this document for an overview of LAMMPS commands for Peridynamics modeling.

For small deformation, dilatation of is the measure of the volumetric strain.

The dilatation "theta" for each peridynamic particle I is calculated as a sum over its neighbors with unbroken bonds, where the contribution of the IJ pair is a function of the change in bond length (versus the initial length in the reference state), the volume fraction of the particles and an influence function. See the PDLAMMPS user guide for a formal definition of dilatation.

This command can only be used with a subset of the Peridynamic *pair styles*: peri/lps, peri/ves and peri/eps.

The dilatation value will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values are unitless numbers (theta) >= 0.0.

17.25.4 Restrictions

This compute is part of the PERI package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.25.5 Related commands

compute damage/atom, *compute plasticity/atom*

Default: none

17.26 compute dipole/chunk command

17.26.1 Syntax

```
compute ID group-ID dipole/chunk chunkID charge-correction
```

- ID, group-ID are documented in *compute* command
- dipole/chunk = style name of this compute command
- chunkID = ID of *compute chunk/atom* command
- charge-correction = *mass* or *geometry*, use COM or geometric center for charged chunk correction (optional)

17.26.2 Examples

```
compute 1 fluid dipole/chunk molchunk
compute dw water dipole/chunk 1 geometry
```

17.26.3 Description

Define a computation that calculates the dipole vector and total dipole for multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a *compute chunk/atom* command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the *compute chunk/atom* and *Howto chunk* doc pages for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

This compute calculates the x,y,z coordinates of the dipole vector and the total dipole moment for each chunk, which includes all effects due to atoms passing through periodic boundaries. For chunks with a net charge the resulting dipole is made position independent by subtracting the position vector of the center of mass or geometric center times the net charge from the computed dipole vector.

Note that only atoms in the specified group contribute to the calculation. The *compute chunk/atom* command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

Note: The coordinates of an atom contribute to the chunk's dipole in "unwrapped" form, by using the image flags associated with each atom. See the *dump custom* command for a discussion of "unwrapped" coordinates. See the Atoms section of the *read_data* command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the *set image* command.

The simplest way to output the results of the compute com/chunk calculation to a file is to use the *fix ave/time* command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all dipole/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk[*] file tmp.out mode vector
```

Output info:

This compute calculates a global array where the number of rows = the number of chunks *Nchunk* as calculated by the specified *compute chunk/atom* command. The number of columns = 4 for the x,y,z dipole vector components and

the total dipole of each chunk. These values can be accessed by any command that uses global array values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The array values are "intensive". The array values will be in dipole units, i.e. charge units times distance *units*.

17.26.4 Restrictions

none

17.26.5 Related commands

compute com/chunk

Default: none

17.27 compute displace/atom command

17.27.1 Syntax

```
compute ID group-ID displace/atom
```

- ID, group-ID are documented in *compute* command
- displace/atom = style name of this compute command
- zero or more keyword/arg pairs may be appended
- keyword = *refresh*

  replace arg = name of per-atom variable

17.27.2 Examples

```
compute 1 all displace/atom
compute 1 all displace/atom refresh myVar
```

17.27.3 Description

Define a computation that calculates the current displacement of each atom in the group from its original (reference) coordinates, including all effects due to atoms passing through periodic boundaries.

A vector of four quantities per atom is calculated by this compute. The first 3 elements of the vector are the dx,dy,dz displacements. The 4th component is the total displacement, i.e. sqrt(dx*dx + dy*dy + dz*dz).

The displacement of an atom is from its original position at the time the compute command was issued. The value of the displacement will be 0.0 for atoms not in the specified compute group.

Note: Initial coordinates are stored in "unwrapped" form, by using the image flags associated with each atom. See the *dump custom* command for a discussion of "unwrapped" coordinates. See the Atoms section of the *read_data*

command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the *set image* command.

Note: If you want the quantities calculated by this compute to be continuous when running from a *restart file*, then you should use the same ID for this compute, as in the original run. This is so that the fix this compute creates to store per-atom quantities will also have the same ID, and thus be initialized correctly with time=0 atom coordinates from the restart file.

The *refresh* option can be used in conjunction with the "dump_modify refresh" command to generate incremental dump files.

The definition and motivation of an incremental dump file is as follows. Instead of outputting all atoms at each snapshot (with some associated values), you may only wish to output the subset of atoms with a value that has changed in some way compared to the value the last time that atom was output. In some scenarios this can result in a dramatically smaller dump file. If desired, by post-processing the sequence of snapshots, the values for all atoms at all timesteps can be inferred.

A concrete example using this compute, is a simulation of atom diffusion in a solid, represented as atoms on a lattice. Diffusive hops are rare. Imagine that when a hop occurs an atom moves more than a distance *Dhop*. For any snapshot we only want to output atoms that have hopped since the last snapshot. This can be accomplished with something like the following commands:

```
write_dump      all custom tmp.dump id type x y z    # see comment below

variable        Dhop equal 0.6
variable        check atom "c_dsp[4] > v_Dhop"
compute         dsp all displace/atom refresh check
dump            1 all custom 100 tmp.dump id type x y z
dump_modify     1 append yes thresh c_dsp[4] > ${Dhop} &
                refresh c_dsp delay 100
```

The *dump_modify thresh* command will only output atoms that have displaced more than 0.6 Angstroms on each snapshot (assuming metal units). The dump_modify *refresh* option triggers a call to this compute at the end of every dump.

The *refresh* argument for this compute is the ID of an *atom-style variable* which calculates a Boolean value (0 or 1) based on the same criterion used by dump_modify thresh. This compute evaluates the atom-style variable. For each atom that returns 1 (true), the original (reference) coordinates of the atom (stored by this compute) are updated.

The effect of these commands is that a particular atom will only be output in the dump file on the snapshot after it makes a diffusive hop. It will not be output again until it makes another hop.

Note that in the first snapshot of a subsequent run, no atoms will be typically be output. That is because the initial displacement for all atoms is 0.0. If an initial dump snapshot is desired, containing the initial reference positions of all atoms, one way to do this is illustrated above. An initial write_dump command can be used before the first run. It will contain the positions of all the atoms, Options in the *dump_modify* command above will append new output to that same file and delay the output until a later timestep. The *delay* setting avoids a second time = 0 snapshot which would be empty.

Output info:

This compute calculates a per-atom array with 4 columns, which can be accessed by indices 1-4 by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom array values will be in distance *units*.

This compute supports the *refresh* option as explained above, for use in conjunction with *dump_modify refresh* to generate incremental dump files.

17.27.4 Restrictions

none

17.27.5 Related commands

compute msd, *dump custom*, *fix store/state*

Default: none

17.28 compute dpd command

17.28.1 Syntax

```
compute ID group-ID dpd
```

- ID, group-ID are documented in *compute* command
- dpd = style name of this compute command

17.28.2 Examples

```
compute 1 all dpd
```

17.28.3 Description

Define a computation that accumulates the total internal conductive energy (U^{cond}), the total internal mechanical energy (U^{mech}), the total chemical energy (U^{chem}) and the *harmonic* average of the internal temperature (θ_{avg}) for the entire system of particles. See the *compute dpd/atom* command if you want per-particle internal energies and internal temperatures.

The system internal properties are computed according to the following relations:

$$
\begin{aligned}
U^{cond} &= \sum_{i=1}^{N} u_i^{cond} \\
U^{mech} &= \sum_{i=1}^{N} u_i^{mech} \\
U^{chem} &= \sum_{i=1}^{N} u_i^{chem} \\
U &= \sum_{i=1}^{N} (u_i^{cond} + u_i^{mech} + u_i^{chem}) \\
\theta_{avg} &= (\frac{1}{N} \sum_{i=1}^{N} \frac{1}{\theta_i})^{-1}
\end{aligned}
$$

where N is the number of particles in the system

Output info:

This compute calculates a global vector of length 5 (U^{cond}, U^{mech}, U^{chem}, θ_{avg}, N), which can be accessed by indices 1-5. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector values will be in energy and temperature *units*.

17.28.4 Restrictions

This command is part of the USER-DPD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This command also requires use of the *atom_style dpd* command.

17.28.5 Related commands

compute dpd/atom, *thermo_style*

Default: none

(Larentzos) J.P. Larentzos, J.K. Brennan, J.D. Moore, and W.D. Mattson, "LAMMPS Implementation of Constant Energy Dissipative Particle Dynamics (DPD-E)", ARL-TR-6863, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD (2014).

17.29 compute dpd/atom command

17.29.1 Syntax

```
compute ID group-ID dpd/atom
```

- ID, group-ID are documented in *compute* command
- dpd/atom = style name of this compute command

17.29.2 Examples

compute 1 all dpd/atom

17.29.3 Description

Define a computation that accesses the per-particle internal conductive energy (u^{cond}), internal mechanical energy (u^{mech}), internal chemical energy (u^{chem}) and internal temperatures (θ) for each particle in a group. See the *compute dpd* command if you want the total internal conductive energy, the total internal mechanical energy, the total chemical energy and average internal temperature of the entire system or group of dpd particles.

Output info:

This compute calculates a per-particle array with 4 columns (u^{cond}, u^{mech}, u^{chem}, θ), which can be accessed by indices 1-4 by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-particle array values will be in energy (u^{cond}, u^{mech}, u^{chem}) and temperature ($theta$) *units*.

17.29.4 Restrictions

This command is part of the USER-DPD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This command also requires use of the *atom_style dpd* command.

17.29.5 Related commands

dump custom, *compute dpd*

Default: none

(Larentzos) J.P. Larentzos, J.K. Brennan, J.D. Moore, and W.D. Mattson, "LAMMPS Implementation of Constant Energy Dissipative Particle Dynamics (DPD-E)", ARL-TR-6863, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD (2014).

17.30 compute edpd/temp/atom command

17.30.1 Syntax

```
compute ID group-ID edpd/temp/atom
```

- ID, group-ID are documented in *compute* command
- edpd/temp/atom = style name of this compute command

17.30.2 Examples

```
compute 1 all edpd/temp/atom
```

17.30.3 Description

Define a computation that calculates the per-atom temperature for each eDPD particle in a group.

The temperature is a local temperature derived from the internal energy of each eDPD particle based on the local equilibrium hypothesis. For more details please see *(Espanol1997)* and *(Li2014)*.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values will be in temperature *units*.

17.30.4 Restrictions

This compute is part of the USER-MESO package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.30.5 Related commands

pair_style edpd

Default: none

(Espanol1997) Espanol, Europhys Lett, 40(6): 631-636 (1997). DOI: 10.1209/epl/i1997-00515-8

(Li2014) Li, Tang, Lei, Caswell, Karniadakis, J Comput Phys, 265: 113-127 (2014). DOI: 10.1016/j.jcp.2014.02.003.

17.31 compute entropy/atom command

17.31.1 Syntax

```
compute ID group-ID entropy/atom sigma cutoff keyword value ...
```

- ID, group-ID are documented in *compute* command
- entropy/atom = style name of this compute command
- sigma = width of gaussians used in the g(r) smoothing
- cutoff = cutoff for the g(r) calculation
- one or more keyword/value pairs may be appended

```
keyword = avg or local
  avg values = yes or no cutoff2
    yes = average the pair entropy over neighbors
    no = do not average the pair entropy over neighbors
    cutoff2 = cutoff for the averaging over neighbors
  local values = yes or no = use the local density around each atom to␣
↪normalize the g(r)
```

17.31.2 Examples

```
compute 1 all entropy/atom 0.25 5.
compute 1 all entropy/atom 0.25 5. avg yes 5.
compute 1 all entropy/atom 0.125 7.3 avg yes 5.1 local yes
```

17.31.3 Description

Define a computation that calculates the pair entropy fingerprint for each atom in the group. The fingerprint is useful to distinguish between ordered and disordered environments, for instance liquid and solid-like environments, or glassy and crystalline-like environments. Some applications could be the identification of grain boundaries, a melt-solid interface, or a solid cluster emerging from the melt. The advantage of this parameter over others is that no a priori information about the solid structure is required.

This parameter for atom i is computed using the following formula from *(Piaggi)* and *(Nettleton)* ,

$$s_S^i = -2\pi\rho k_B \int_0^{r_m} \left[g(r)\ln g(r) - g(r) + 1\right] r^2 dr$$

where r is a distance, g(r) is the radial distribution function of atom i and rho is the density of the system. The g(r) computed for each atom i can be noisy and therefore it is smoothed using:

$$g_m^i(r) = \frac{1}{4\pi\rho r^2} \sum_j \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(r-r_{ij})^2/(2\sigma^2)}$$

where the sum in j goes through the neighbors of atom i, and σ is a parameter to control the smoothing.

The input parameters are *sigma* the smoothing parameter σ, and the *cutoff* for the calculation of g(r).

If the keyword *avg* has the setting *yes*, then this compute also averages the parameter over the neighbors of atom i according to:

$$\left\langle s_S^i \right\rangle = \frac{\sum_j s_S^j + s_S^i}{N+1}$$

where the sum j goes over the neighbors of atom i and N is the number of neighbors. This procedure provides a sharper distinction between order and disorder environments. In this case the input parameter *cutoff2* is the cutoff for the averaging over the neighbors and must also be specified.

If the *avg yes* option is used, the effective cutoff of the neighbor list should be *cutoff*+*cutoff2* and therefore it might be necessary to increase the skin of the neighbor list with:

```
neighbor skin bin
```

See *neighbor* for details.

If the *local yes* option is used, the g(r) is normalized by the local density around each atom, that is to say the density around each atom is the number of neighbors within the neighbor list cutoff divided by the corresponding volume. This option can be useful when dealing with inhomogeneous systems such as those that have surfaces.

Here are typical input parameters for fcc aluminum (lattice constant 4.05 Angstroms),

```
compute 1 all entropy/atom 0.25 5.7 avg yes 3.7
```

and for bcc sodium (lattice constant 4.23 Angstroms),

```
compute 1 all entropy/atom 0.25 7.3 avg yes 5.1
```

Output info:

By default, this compute calculates the pair entropy value for each atom as a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The pair entropy values have units of the Boltzmann constant. They are always negative, and lower values (lower entropy) correspond to more ordered environments.

17.31.4 Restrictions

This compute is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.31.5 Related commands

compute cna/atom compute centro/atom

17.31.6 Default

The default values for the optional keywords are avg = no and local = no.

(Piaggi) Piaggi and Parrinello, J Chem Phys, 147, 114112 (2017).

(Nettleton) Nettleton and Green, J Chem Phys, 29, 6 (1958).

17.32 compute erotate/asphere command

17.32.1 Syntax

```
compute ID group-ID erotate/asphere
```

- ID, group-ID are documented in *compute* command
- erotate/asphere = style name of this compute command

17.32.2 Examples

```
compute 1 all erotate/asphere
```

17.32.3 Description

Define a computation that calculates the rotational kinetic energy of a group of aspherical particles. The aspherical particles can be ellipsoids, or line segments, or triangles. See the *atom_style* and *read_data* commands for descriptions of these options.

For all 3 types of particles, the rotational kinetic energy is computed as 1/2 I w^2, where I is the inertia tensor for the aspherical particle and w is its angular velocity, which is computed from its angular momentum if needed.

Note: For *2d models*, ellipsoidal particles are treated as ellipsoids, not ellipses, meaning their moments of inertia will be the same as in 3d.

Output info:

This compute calculates a global scalar (the KE). This value can be used by any command that uses a global scalar value from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy *units*.

17.32.4 Restrictions

This compute requires that ellipsoidal particles atoms store a shape and quaternion orientation and angular momentum as defined by the *atom_style ellipsoid* command.

This compute requires that line segment particles atoms store a length and orientation and angular velocity as defined by the *atom_style line* command.

This compute requires that triangular particles atoms store a size and shape and quaternion orientation and angular momentum as defined by the *atom_style tri* command.

All particles in the group must be finite-size. They cannot be point particles.

Related commands: none

compute erotate/sphere

Default: none

17.33 compute erotate/rigid command

17.33.1 Syntax

```
compute ID group-ID erotate/rigid fix-ID
```

- ID, group-ID are documented in *compute* command
- erotate/rigid = style name of this compute command
- fix-ID = ID of rigid body fix

17.33.2 Examples

```
compute 1 all erotate/rigid myRigid
```

17.33.3 Description

Define a computation that calculates the rotational kinetic energy of a collection of rigid bodies, as defined by one of the *fix rigid* command variants.

The rotational energy of each rigid body is computed as 1/2 I Wbody^2, where I is the inertia tensor for the rigid body, and Wbody is its angular velocity vector. Both I and Wbody are in the frame of reference of the rigid body, i.e. I is diagonalized.

The *fix-ID* should be the ID of one of the *fix rigid* commands which defines the rigid bodies. The group specified in the compute command is ignored. The rotational energy of all the rigid bodies defined by the fix rigid command in included in the calculation.

Output info:

This compute calculates a global scalar (the summed rotational energy of all the rigid bodies). This value can be used by any command that uses a global scalar value from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy *units*.

17.33.4 Restrictions

This compute is part of the RIGID package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.33.5 Related commands

compute ke/rigid

Default: none

17.34 compute erotate/sphere command

17.34.1 Syntax

```
compute ID group-ID erotate/sphere
```

- ID, group-ID are documented in *compute* command
- erotate/sphere = style name of this compute command

17.34.2 Examples

```
compute 1 all erotate/sphere
```

17.34.3 Description

Define a computation that calculates the rotational kinetic energy of a group of spherical particles.

The rotational energy is computed as 1/2 I w^2, where I is the moment of inertia for a sphere and w is the particle's angular velocity.

Note: For *2d models*, particles are treated as spheres, not disks, meaning their moment of inertia will be the same as in 3d.

Output info:

This compute calculates a global scalar (the KE). This value can be used by any command that uses a global scalar value from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy *units*.

17.34.4 Restrictions

This compute requires that atoms store a radius and angular velocity (omega) as defined by the *atom_style sphere* command.

All particles in the group must be finite-size spheres or point particles. They cannot be aspherical. Point particles will not contribute to the rotational energy.

17.34.5 Related commands

compute erotate/asphere

Default: none

17.35 compute erotate/sphere/atom command

17.35.1 Syntax

```
compute ID group-ID erotate/sphere/atom
```

- ID, group-ID are documented in *compute* command
- erotate/sphere/atom = style name of this compute command

17.35.2 Examples

```
compute 1 all erotate/sphere/atom
```

17.35.3 Description

Define a computation that calculates the rotational kinetic energy for each particle in a group.

The rotational energy is computed as 1/2 I w^2, where I is the moment of inertia for a sphere and w is the particle's angular velocity.

Note: For *2d models*, particles are treated as spheres, not disks, meaning their moment of inertia will be the same as in 3d.

The value of the rotational kinetic energy will be 0.0 for atoms not in the specified compute group or for point particles with a radius = 0.0.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values will be in energy *units*.

17.35.4 Restrictions

none

17.35.5 Related commands

dump custom

Default: none

17.36 compute event/displace command

17.36.1 Syntax

```
compute ID group-ID event/displace threshold
```

- ID, group-ID are documented in *compute* command
- event/displace = style name of this compute command
- threshold = minimum distance any particle must move to trigger an event (distance units)

17.36.2 Examples

```
compute 1 all event/displace 0.5
```

17.36.3 Description

Define a computation that flags an "event" if any particle in the group has moved a distance greater than the specified threshold distance when compared to a previously stored reference state (i.e. the previous event). This compute is typically used in conjunction with the *prd* and *tad* commands, to detect if a transition to a new minimum energy basin has occurred.

This value calculated by the compute is equal to 0 if no particle has moved far enough, and equal to 1 if one or more particles have moved further than the threshold distance.

Note: If the system is undergoing significant center-of-mass motion, due to thermal motion, an external force, or an initial net momentum, then this compute will not be able to distinguish that motion from local atom displacements and may generate "false positives."

Output info:

This compute calculates a global scalar (the flag). This value can be used by any command that uses a global scalar value from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The scalar value will be a 0 or 1 as explained above.

17.36.4 Restrictions

This command can only be used if LAMMPS was built with the REPLICA package. See the *Build package* doc page for more info.

17.36.5 Related commands

prd, *tad*

Default: none

17.37 compute fep command

17.37.1 Syntax

```
compute ID group-ID fep temp attribute args ... keyword value ...
```

- ID, group-ID are documented in the *compute* command
- fep = name of this compute command
- temp = external temperature (as specified for constant-temperature run)
- one or more attributes with args may be appended
- attribute = *pair* or *atom*

```
pair args = pstyle pparam I J v_delta
  pstyle = pair style name, e.g. lj/cut
  pparam = parameter to perturb
  I,J = type pair(s) to set parameter for
  v_delta = variable with perturbation to apply (in the units of the␣
↪parameter)
atom args = aparam I v_delta
  aparam = parameter to perturb
  I = type to set parameter for
  v_delta = variable with perturbation to apply (in the units of the␣
↪parameter)
```

- zero or more keyword/value pairs may be appended
- keyword = *tail* or *volume*

```
tail value = no or yes
  no = ignore tail correction to pair energies (usually small in fep)
  yes = include tail correction to pair energies
volume value = no or yes
  no = ignore volume changes (e.g. in NVE or NVT trajectories)
  yes = include volume changes (e.g. in NpT trajectories)
```

17.37.2 Examples

```
compute 1 all fep 298 pair lj/cut epsilon 1 * v_delta pair lj/cut sigma 1 * v_
↪delta volume yes
compute 1 all fep 300 atom charge 2 v_delta
```

17.37.3 Description

Apply a perturbation to parameters of the interaction potential and recalculate the pair potential energy without changing the atomic coordinates from those of the reference, unperturbed system. This compute can be used to calculate free energy differences using several methods, such as free-energy perturbation (FEP), finite-difference thermodynamic integration (FDTI) or Bennet's acceptance ratio method (BAR).

The potential energy of the system is decomposed in three terms: a background term corresponding to interaction sites whose parameters remain constant, a reference term U_0 corresponding to the initial interactions of the atoms that will undergo perturbation, and a term U_1 corresponding to the final interactions of these atoms:

$$U(\lambda) = U_{\mathrm{bg}} + U_1(\lambda) + U_0(\lambda)$$

A coupling parameter λ varying from 0 to 1 connects the reference and perturbed systems:

$$\begin{aligned} \lambda = 0 \quad &\Rightarrow \quad U = U_{\mathrm{bg}} + U_0 \\ \lambda = 1 \quad &\Rightarrow \quad U = U_{\mathrm{bg}} + U_1 \end{aligned}$$

It is possible but not necessary that the coupling parameter (or a function thereof) appears as a multiplication factor of the potential energy. Therefore, this compute can apply perturbations to interaction parameters that are not directly proportional to the potential energy (e.g. σ in Lennard-Jones potentials).

This command can be combined with *fix adapt* to perform multistage free-energy perturbation calculations along stepwise alchemical transformations during a simulation run:

$$\Delta_0^1 A = \sum_{i=0}^{n-1} \Delta_{\lambda_i}^{\lambda_{i+1}} A = -kT \sum_{i=0}^{n-1} \ln \left\langle \exp\left(-\frac{U(\lambda_{i+1}) - U(\lambda_i)}{kT} \right) \right\rangle_{\lambda_i}$$

This compute is suitable for the finite-difference thermodynamic integration (FDTI) method *(Mezei)*, which is based on an evaluation of the numerical derivative of the free energy by a perturbation method using a very small δ:

$$\Delta_0^1 A = \int_{\lambda=0}^{\lambda=1} \left(\frac{\partial A(\lambda)}{\partial \lambda} \right)_\lambda \mathrm{d}\lambda \approx \sum_{i=0}^{n-1} w_i \frac{A(\lambda_i + \delta) - A(\lambda_i)}{\delta}$$

where w_i are weights of a numerical quadrature. The *fix adapt* command can be used to define the stages of λ at which the derivative is calculated and averaged.

The compute fep calculates the exponential Boltzmann term and also the potential energy difference $U_1 - U_0$. By choosing a very small perturbation δ the thermodynamic integration method can be implemented using a numerical evaluation of the derivative of the potential energy with respect to λ:

$$\Delta_0^1 A = \int_{\lambda=0}^{\lambda=1} \left\langle \frac{\partial U(\lambda)}{\partial \lambda} \right\rangle_\lambda \mathrm{d}\lambda \approx \sum_{i=0}^{n-1} w_i \left\langle \frac{U(\lambda_i + \delta) - U(\lambda_i)}{\delta} \right\rangle_{\lambda_i}$$

Another technique to calculate free energy differences is the acceptance ratio method *(Bennet)*, which can be implemented by calculating the potential energy differences with δ = 1.0 on both the forward and reverse routes:

$$\left\langle \frac{1}{1 + \exp\left[\left(U_1 - U_0 - \Delta_0^1 A\right)/kT\right]} \right\rangle_0 = \left\langle \frac{1}{1 + \exp\left[\left(U_0 - U_1 + \Delta_0^1 A\right)/kT\right]} \right\rangle_1$$

The value of the free energy difference is determined by numerical root finding to establish the equality.

Concerning the choice of how the atomic parameters are perturbed in order to setup an alchemical transformation route, several strategies are available, such as single-topology or double-topology strategies *(Pearlman)*. The latter does not require modification of bond lengths, angles or other internal coordinates.

NOTES: This compute command does not take kinetic energy into account, therefore the masses of the particles should not be modified between the reference and perturbed states, or along the alchemical transformation route. This compute command does not change bond lengths or other internal coordinates *(Boresch, Karplus)*.

The *pair* attribute enables various parameters of potentials defined by the *pair_style* and *pair_coeff* commands to be changed, if the pair style supports it.

The *pstyle* argument is the name of the pair style. For example, *pstyle* could be specified as "lj/cut". The *pparam* argument is the name of the parameter to change. This is a list of pair styles and parameters that can be used with this compute. See the doc pages for individual pair styles and their energy formulas for the meaning of these parameters:

born	a,b,c	type pairs
buck	a,c	type pairs
buck/mdf	a,c	type pairs
coul/cut	scale	type pairs
coul/cut/soft	lambda	type pairs
coul/long, coul/msm	scale	type pairs
coul/long/soft	scale, lambda	type pairs
eam	scale	type pairs
gauss	a	type pairs
lennard/mdf	a,b	type pairs
lj/class2	epsilon,sigma	type pairs
lj/class2/coul/cut, lj/class2/coul/long	epsilon,sigma	type pairs
lj/cut	epsilon,sigma	type pairs
lj/cut/soft	epsilon,sigma,lambda	type pairs
lj/cut/coul/cut, lj/cut/coul/long, lj/cut/coul/msm	epsilon,sigma	type pairs
lj/cut/coul/cut/soft, lj/cut/coul/long/soft	epsilon,sigma,lambda	type pairs
lj/cut/tip4p/cut, lj/cut/tip4p/long	epsilon,sigma	type pairs
lj/cut/tip4p/long/soft	epsilon,sigma,lambda	type pairs
lj/expand	epsilon,sigma,delta	type pairs
lj/mdf	epsilon,sigma	type pairs
lj/sf/dipole/sf	epsilon,sigma,scale	type pairs
mie/cut	epsilon,sigma,gamR,gamA	type pairs
morse, morse/smooth/linear	d0,r0,alpha	type pairs
morse/soft	d0,r0,alpha,lambda	type pairs
nm/cut	e0,r0,nn,mm	type pairs
nm/cut/coul/cut, nm/cut/coul/long	e0,r0,nn,mm	type pairs
ufm	epsilon,sigma,scale	type pairs
soft	a	type pairs

Note that it is easy to add new potentials and their parameters to this list. All it typically takes is adding an extract() method to the pair_*.cpp file associated with the potential.

Similar to the *pair_coeff* command, I and J can be specified in one of two ways. Explicit numeric values can be used for each, as in the 1st example above. I <= J is required. LAMMPS sets the coefficients for the symmetric J,I interaction to the same values. A wild-card asterisk can be used in place of or in conjunction with the I,J arguments to set the coefficients for multiple pairs of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). Note that only type pairs with I <= J are considered; if asterisks imply type pairs where J < I, they are ignored.

If *pair_style hybrid or hybrid/overlay* is being used, then the *pstyle* will be a sub-style name. You must specify I,J arguments that correspond to type pair values defined (via the *pair_coeff* command) for that sub-style.

The *v_name* argument for keyword *pair* is the name of an *equal-style variable* which will be evaluated each time this compute is invoked. It should be specified as v_name, where name is the variable name.

The *atom* attribute enables atom properties to be changed. The *aparam* argument is the name of the parameter to change. This is the current list of atom parameters that can be used with this compute:

- charge = charge on particle

The *v_name* argument for keyword *pair* is the name of an *equal-style variable* which will be evaluated each time this compute is invoked. It should be specified as v_name, where name is the variable name.

The *tail* keyword controls the calculation of the tail correction to "van der Waals" pair energies beyond the cutoff, if this has been activated via the *pair_modify* command. If the perturbation is small, the tail contribution to the energy difference between the reference and perturbed systems should be negligible.

If the keyword *volume* = *yes*, then the Boltzmann term is multiplied by the volume so that correct ensemble averaging can be performed over trajectories during which the volume fluctuates or changes *(Allen and Tildesley)*:

$$\Delta_0^1 A = -kT \sum_{i=0}^{n-1} \ln \frac{\left\langle V \exp\left(-\frac{U(\lambda_{i+1})-U(\lambda_i)}{kT}\right)\right\rangle_{\lambda_i}}{\langle V \rangle_{\lambda_i}}$$

Output info:

This compute calculates a global vector of length 3 which contains the energy difference ($U_1 - U_0$) as c_ID[1], the Boltzmann factor $\exp(-(U_1 - U_0)/kT)$, or $V \exp(-(U_1 - U_0)/kT)$, as c_ID[2] and the volume of the simulation box V as c_ID[3]. U_1 is the pair potential energy obtained with the perturbed parameters and U_0 is the pair potential energy obtained with the unperturbed parameters. The energies include kspace terms if these are used in the simulation.

These output results can be used by any command that uses a global scalar or vector from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options. For example, the computed values can be averaged using *fix ave/time*.

The values calculated by this compute are "extensive".

17.37.4 Restrictions

This compute is distributed as the USER-FEP package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.37.5 Related commands

fix adapt/fep, *fix ave/time*, *pair_style . . . /soft*

17.37.6 Default

The option defaults are *tail* = *no*, *volume* = *no*.

(Pearlman) Pearlman, J Chem Phys, 98, 1487 (1994)

(Mezei) Mezei, J Chem Phys, 86, 7084 (1987)

(Bennet) Bennet, J Comput Phys, 22, 245 (1976)

(BoreschKarplus) Boresch and Karplus, J Phys Chem A, 103, 103 (1999)

(AllenTildesley) Allen and Tildesley, Computer Simulation of Liquids, Oxford University Press (1987)

17.38 compute global/atom command

17.38.1 Syntax

```
compute ID group-ID style index input1 input2 ...
```

- ID, group-ID are documented in *compute* command
- global/atom = style name of this compute command
- index = c_ID, c_ID[N], f_ID, f_ID[N], v_name

```
c_ID = per-atom vector calculated by a compute with ID
c_ID[I] = Ith column of per-atom array calculated by a compute with ID
f_ID = per-atom vector calculated by a fix with ID
f_ID[I] = Ith column of per-atom array calculated by a fix with ID
v_name = per-atom vector calculated by an atom-style variable with name
```

- one or more inputs can be listed
- input = c_ID, c_ID[N], f_ID, f_ID[N], v_name

```
c_ID = global vector calculated by a compute with ID
c_ID[I] = Ith column of global array calculated by a compute with ID, I can␣
↪include wildcard (see below)
f_ID = global vector calculated by a fix with ID
f_ID[I] = Ith column of global array calculated by a fix with ID, I can include␣
↪wildcard (see below)
v_name = global vector calculated by a vector-style variable with name
```

17.38.2 Examples

```
compute 1 all global/atom c_chunk c_com[1] c_com[2] c_com[3]
compute 1 all global/atom c_chunk c_com[*]
```

17.38.3 Description

Define a calculation that assigns global values to each atom from vectors or arrays of global values. The specified *index* parameter is used to determine which global value is assigned to each atom.

The *index* parameter must reference a per-atom vector or array from a *compute* or *fix* or the evaluation of an atom-style *variable*. Each *input* value must reference a global vector or array from a *compute* or *fix* or the evaluation of an vector-style *variable*. Details are given below.

The *index* value for an atom is used as a index I (from 1 to N) into the vector associated with each of the input values. The Ith value from the input vector becomes one output value for that atom. If the atom is not in the specified group, or the index I < 1 or I > M, where M is the actual length of the input vector, then an output value of 0.0 is assigned to the atom.

An example of how this command is useful, is in the context of "chunks" which are static or dynamic subsets of atoms. The *compute chunk/atom* command assigns unique chunk IDs to each atom. It's output can be used as the *index* parameter for this command. Various other computes with "chunk" in their style name, such as *compute com/chunk* or *compute msd/chunk*, calculate properties for each chunk. The output of these commands are global vectors or arrays, with one or more values per chunk, and can be used as input values for this command. This command will then assign the global chunk value to each atom in the chunk, producing a per-atom vector or per-atom array as output. The

per-atom values can then be output to a dump file or used by any command that uses per-atom values from a compute as input, as discussed on the *Howto output* doc page.

As a concrete example, these commands will calculate the displacement of each atom from the center-of-mass of the molecule it is in, and dump those values to a dump file. In this case, each molecule is a chunk.

```
compute cc1 all chunk/atom molecule
compute myChunk all com/chunk cc1
compute prop all property/atom xu yu zu
compute glob all global/atom c_cc1 c_myChunk[*]
variable dx atom c_prop[1]-c_glob[1]
variable dy atom c_prop[2]-c_glob[2]
variable dz atom c_prop[3]-c_glob[3]
variable dist atom sqrt(v_dx*v_dx+v_dy*v_dy+v_dz*v_dz)
dump 1 all custom 100 tmp.dump id xu yu zu c_glob[1] c_glob[2] c_glob[3] &
     v_dx v_dy v_dz v_dist
dump_modify 1 sort id
```

You can add these commands to the bench/in.chain script to see how they work.

Note that for input values from a compute or fix, the bracketed index I can be specified using a wildcard asterisk with the index to effectively specify multiple values. This takes the form "*" or "*n" or "n*" or "m*n". If N = the size of the vector (for *mode* = scalar) or the number of columns in the array (for *mode* = vector), then an asterisk with no numeric values means all indices from 1 to N. A leading asterisk means all indices from 1 to n (inclusive). A trailing asterisk means all indices from n to N (inclusive). A middle asterisk means all indices from m to n (inclusive).

Using a wildcard is the same as if the individual columns of the array had been listed one by one. E.g. these 2 compute global/atom commands are equivalent, since the *compute com/chunk* command creates a global array with 3 columns:

```
compute cc1 all chunk/atom molecule
compute com all com/chunk cc1
compute 1 all global/atom c_cc1 c_com[1] c_com[2] c_com[3]
compute 1 all global/atom c_cc1 c_com[*]
```

This section explains the *index* parameter. Note that it must reference per-atom values, as contrasted with the *input* values which must reference global values.

Note that all of these options generate floating point values. When they are used as an index into the specified input vectors, they simple rounded down to convert the value to integer indices. The final values should range from 1 to N (inclusive), since they are used to access values from N-length vectors.

If *index* begins with "c_", a compute ID must follow which has been previously defined in the input script. The compute must generate per-atom quantities. See the individual *compute* doc page for details. If no bracketed integer is appended, the per-atom vector calculated by the compute is used. If a bracketed integer is appended, the Ith column of the per-atom array calculated by the compute is used. Users can also write code for their own compute styles and *add them to LAMMPS*. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

If *index* begins with "f_", a fix ID must follow which has been previously defined in the input script. The Fix must generate per-atom quantities. See the individual *fix* doc page for details. Note that some fixes only produce their values on certain timesteps, which must be compatible with when compute global/atom references the values, else an error results. If no bracketed integer is appended, the per-atom vector calculated by the fix is used. If a bracketed integer is appended, the Ith column of the per-atom array calculated by the fix is used. Users can also write code for their own fix style and *add them to LAMMPS*. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

If *index* begins with "v_", a variable name must follow which has been previously defined in the input script. It must be an *atom-style variable*. Atom-style variables can reference thermodynamic keywords and various per-atom attributes, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of generating per-atom quantities to use as *index*.

This section explains the kinds of *input* values that can be used. Note that inputs reference global values, as contrasted with the *index* parameter which must reference per-atom values.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. The compute must generate a global vector or array. See the individual *compute* doc page for details. If no bracketed integer is appended, the vector calculated by the compute is used. If a bracketed integer is appended, the Ith column of the array calculated by the compute is used. Users can also write code for their own compute styles and *add them to LAMMPS*. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. The fix must generate a global vector or array. See the individual *fix* doc page for details. Note that some fixes only produce their values on certain timesteps, which must be compatible with when compute global/atom references the values, else an error results. If no bracketed integer is appended, the vector calculated by the fix is used. If a bracketed integer is appended, the Ith column of the array calculated by the fix is used. Users can also write code for their own fix style and *add them to LAMMPS*. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. It must be a *vector-style variable*. Vector-style variables can reference thermodynamic keywords and various other attributes of atoms, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of generating a vector of global quantities which the *index* parameter will reference for assignment of global values to atoms.

Output info:

If a single input is specified this compute produces a per-atom vector. If multiple inputs are specified, this compute produces a per-atom array values, where the number of columns is equal to the number of inputs specified. These values can be used by any command that uses per-atom vector or array values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector or array values will be in whatever units the corresponding input values are in.

17.38.4 Restrictions

none

17.38.5 Related commands

compute, *fix*, *variable*, *compute chunk/atom*, *compute reduce*

Default: none

17.39 compute group/group command

17.39.1 Syntax

```
compute ID group-ID group/group group2-ID keyword value ...
```

- ID, group-ID are documented in *compute* command
- group/group = style name of this compute command
- group2-ID = group ID of second (or same) group
- zero or more keyword/value pairs may be appended
- keyword = *pair* or *kspace* or *boundary* or *molecule*

  pair value = *yes* or *no*
  kspace value = *yes* or *no*
  boundary value = *yes* or *no*
  molecule value = *off* or *inter* or *intra*

17.39.2 Examples

```
compute 1 lower group/group upper
compute 1 lower group/group upper kspace yes
compute mine fluid group/group wall
```

17.39.3 Description

Define a computation that calculates the total energy and force interaction between two groups of atoms: the compute group and the specified group2. The two groups can be the same.

If the *pair* keyword is set to *yes*, which is the default, then the the interaction energy will include a pair component which is defined as the pairwise energy between all pairs of atoms where one atom in the pair is in the first group and the other is in the second group. Likewise, the interaction force calculated by this compute will include the force on the compute group atoms due to pairwise interactions with atoms in the specified group2.

Note: The energies computed by the *pair* keyword do not include tail corrections, even if they are enabled via the *pair_modify* command.

If the *molecule* keyword is set to *inter* or *intra* than an additional check is made based on the molecule IDs of the two atoms in each pair before including their pairwise interaction energy and force. For the *inter* setting, the two atoms must be in different molecules. For the *intra* setting, the two atoms must be in the same molecule.

If the *kspace* keyword is set to *yes*, which is not the default, and if a *kspace_style* is defined, then the interaction energy will include a Kspace component which is the long-range Coulombic energy between all the atoms in the first group and all the atoms in the 2nd group. Likewise, the interaction force calculated by this compute will include the force on the compute group atoms due to long-range Coulombic interactions with atoms in the specified group2.

Normally the long-range Coulombic energy converges only when the net charge of the unit cell is zero. However, one can assume the net charge of the system is neutralized by a uniform background plasma, and a correction to the system energy can be applied to reduce artifacts. For more information see *(Bogusz)*. If the *boundary* keyword is set to *yes*, which is the default, and *kspace* contributions are included, then this energy correction term will be added to the total

group-group energy. This correction term does not affect the force calculation and will be zero if one or both of the groups are charge neutral. This energy correction term is the same as that included in the regular Ewald and PPPM routines.

Note: The *molecule* setting only affects the group/group contributions calculated by the *pair* keyword. It does not affect the group/group contributions calculated by the *kspace* keyword.

This compute does not calculate any bond or angle or dihedral or improper interactions between atoms in the two groups.

The pairwise contributions to the group-group interactions are calculated by looping over a neighbor list. The Kspace contribution to the group-group interactions require essentially the same amount of work (FFTs, Ewald summation) as computing long-range forces for the entire system. Thus it can be costly to invoke this compute too frequently.

Note: If you have a bonded system, then the settings of *special_bonds* command can remove pairwise interactions between atoms in the same bond, angle, or dihedral. This is the default setting for the *special_bonds* command, and means those pairwise interactions do not appear in the neighbor list. Because this compute uses a neighbor list, it also means those pairs will not be included in the group/group interaction. This does not apply when using long-range coulomb interactions (*coul/long*, *coul/msm*, *coul/wolf* or similar. One way to get around this would be to set special_bond scaling factors to very tiny numbers that are not exactly zero (e.g. 1.0e-50). Another workaround is to write a dump file, and use the *rerun* command to compute the group/group interactions for snapshots in the dump file. The rerun script can use a *special_bonds* command that includes all pairs in the neighbor list.

If you desire a breakdown of the interactions into a pairwise and Kspace component, simply invoke the compute twice with the appropriate yes/no settings for the *pair* and *kspace* keywords. This is no more costly than using a single compute with both keywords set to *yes*. The individual contributions can be summed in a *variable* if desired.

This document describes how the long-range group-group calculations are performed.

Output info:

This compute calculates a global scalar (the energy) and a global vector of length 3 (force), which can be accessed by indices 1-3. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

Both the scalar and vector values calculated by this compute are "extensive". The scalar value will be in energy *units*. The vector values will be in force *units*.

17.39.4 Restrictions

Not all pair styles can be evaluated in a pairwise mode as required by this compute. For example, 3-body and other many-body potentials, such as *Tersoff* and *Stillinger-Weber* cannot be used. *EAM* potentials will re-use previously computed embedding term contributions, so the computed pairwise forces and energies are based on the whole system and not valid if particles have been moved since.

Not all *Kspace styles* support the calculation of group/group interactions. The regular *ewald* and *pppm* styles do.

Related commands: none

17.39.5 Default

The option defaults are pair = yes, kspace = no, boundary = yes, molecule = off.

Bogusz et al, J Chem Phys, 108, 7070 (1998)

17.40 compute gyration command

17.40.1 Syntax

```
compute ID group-ID gyration
```

- ID, group-ID are documented in *compute* command
- gyration = style name of this compute command

17.40.2 Examples

```
compute 1 molecule gyration
```

17.40.3 Description

Define a computation that calculates the radius of gyration Rg of the group of atoms, including all effects due to atoms passing through periodic boundaries.

Rg is a measure of the size of the group of atoms, and is computed as the square root of the Rg^2 value in this formula

$$R_g{}^2 = \frac{1}{M} \sum_i m_i (r_i - r_{cm})^2$$

where M is the total mass of the group, r_{cm} is the center-of-mass position of the group, and the sum is over all atoms in the group.

A $R_g{}^2$ tensor, stored as a 6-element vector, is also calculated by this compute. The formula for the components of the tensor is the same as the above formula, except that $(r_i - r_{cm})^2$ is replaced by $(r_{i,x} - r_{cm,x}) \cdot (r_{i,y} - r_{cm,y})$ for the xy component, and so on. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz. Note that unlike the scalar R_g, each of the 6 values of the tensor is effectively a "squared" value, since the cross-terms may be negative and taking a sqrt() would be invalid.

Note: The coordinates of an atom contribute to R_g in "unwrapped" form, by using the image flags associated with each atom. See the *dump custom* command for a discussion of "unwrapped" coordinates. See the Atoms section of the *read_data* command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the *set image* command.

Output info:

This compute calculates a global scalar (R_g) and a global vector of length 6 ($R_g{}^2$ tensor), which can be accessed by indices 1-6. These values can be used by any command that uses a global scalar value or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar and vector values calculated by this compute are "intensive". The scalar and vector values will be in distance and distance^2 *units* respectively.

17.40.4 Restrictions

none

17.40.5 Related commands

compute gyration/chunk, *compute gyration/shape*

Default: none

17.41 compute gyration/chunk command

17.41.1 Syntax

```
compute ID group-ID gyration/chunk chunkID keyword value ...
```

- ID, group-ID are documented in *compute* command
- gyration/chunk = style name of this compute command
- chunkID = ID of *compute chunk/atom* command
- zero or more keyword/value pairs may be appended
- keyword = *tensor*

  tensor value = none

17.41.2 Examples

```
compute 1 molecule gyration/chunk molchunk
compute 2 molecule gyration/chunk molchunk tensor
```

17.41.3 Description

Define a computation that calculates the radius of gyration Rg for multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a *compute chunk/atom* command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the *compute chunk/atom* and *Howto chunk* doc pages for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

This compute calculates the radius of gyration Rg for each chunk, which includes all effects due to atoms passing through periodic boundaries.

Rg is a measure of the size of a chunk, and is computed by this formula

$$R_g{}^2 = \frac{1}{M} \sum_i m_i (r_i - r_{cm})^2$$

where M is the total mass of the chunk, r_{cm} is the center-of-mass position of the chunk, and the sum is over all atoms in the chunk.

Note that only atoms in the specified group contribute to the calculation. The *compute chunk/atom* command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

If the *tensor* keyword is specified, then the scalar Rg value is not calculated, but an Rg tensor is instead calculated for each chunk. The formula for the components of the tensor is the same as the above formula, except that $(r_i - r_{cm})^2$ is replaced by $(r_{i,x} - r_{cm,x}) \cdot (r_{i,y} - r_{cm,y})$ for the xy component, and so on. The 6 components of the tensor are ordered xx, yy, zz, xy, xz, yz.

Note: The coordinates of an atom contribute to R_g in "unwrapped" form, by using the image flags associated with each atom. See the *dump custom* command for a discussion of "unwrapped" coordinates. See the Atoms section of the *read_data* command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the *set image* command.

The simplest way to output the results of the compute gyration/chunk calculation to a file is to use the *fix ave/time* command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all gyration/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk file tmp.out mode vector
```

Output info:

This compute calculates a global vector if the *tensor* keyword is not specified and a global array if it is. The length of the vector or number of rows in the array = the number of chunks *Nchunk* as calculated by the specified *compute chunk/atom* command. If the *tensor* keyword is specified, the global array has 6 columns. The vector or array can be accessed by any command that uses global values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

All the vector or array values calculated by this compute are "intensive". The vector or array values will be in distance *units*, since they are the square root of values represented by the formula above.

17.41.4 Restrictions

none

Related commands: none

compute gyration

Default: none

17.42 compute gyration/shape command

17.42.1 Syntax

```
compute ID group-ID gyration/shape compute-ID
```

- ID, group-ID are documented in *compute* command
- gyration/shape = style name of this compute command
- compute-ID = ID of *compute gyration* command

17.42.2 Examples

```
compute 1 molecule gyration/shape pe
```

17.42.3 Description

Define a computation that calculates the eigenvalues of the gyration tensor of a group of atoms and three shape parameters. The computation includes all effects due to atoms passing through periodic boundaries.

The three computed shape parameters are the asphericity, b, the acylindricity, c, and the relative shape anisotropy, k:

$$\begin{aligned} c =& l_z - 0.5(l_y + l_x) \\ b =& l_y - l_x \\ k =& \frac{3}{2}\frac{l_x^2 + l_y^2 + l_z^2}{(l_x + l_y + l_z)^2} - \frac{1}{2} \end{aligned}$$

where l_x <= l_y <= l_z are the three eigenvalues of the gyration tensor. A general description of these parameters is provided in *(Mattice)* while an application to polymer systems can be found in *(Theodorou)*. The asphericity is always non-negative and zero only when the three principal moments are equal. This zero condition is met when the distribution of particles is spherically symmetric (hence the name asphericity) but also whenever the particle distribution is symmetric with respect to the three coordinate axes, e.g., when the particles are distributed uniformly on a cube, tetrahedron or other Platonic solid. The acylindricity is always non-negative and zero only when the two principal moments are equal. This zero condition is met when the distribution of particles is cylindrically symmetric (hence the name, acylindricity), but also whenever the particle distribution is symmetric with respect to the two coordinate axes, e.g., when the particles are distributed uniformly on a regular prism. the relative shape anisotropy is bounded between zero (if all points are spherically symmetric) and one (if all points lie on a line).

Note: The coordinates of an atom contribute to the gyration tensor in "unwrapped" form, by using the image flags associated with each atom. See the *dump custom* command for a discussion of "unwrapped" coordinates. See the Atoms section of the *read_data* command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the *set image* command.

Output info:

This compute calculates a global vector of length 6, which can be accessed by indices 1-6. The first three values are the eigenvalues of the gyration tensor followed by the asphericity, the acylindricity and the relative shape anisotropy. The computed values can be used by any command that uses global vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector values calculated by this compute are "intensive". The first five vector values will be in distance^2 *units* while the sixth one is dimensionless.

17.42.4 Restrictions

This compute is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.42.5 Related commands

compute gyration

Default: none

(Mattice) Mattice, Suter, Conformational Theory of Large Molecules, Wiley, New York, 1994.

(Theodorou) Theodorou, Suter, Macromolecules, 18, 1206 (1985).

17.43 compute gyration/shape/chunk command

17.43.1 Syntax

```
compute ID group-ID gyration/shape/chunk compute-ID
```

- ID, group-ID are documented in *compute* command
- gyration/shape/chunk = style name of this compute command
- compute-ID = ID of *compute gyration/chunk* command

17.43.2 Examples

```
compute 1 molecule gyration/shape/chunk pe
```

17.43.3 Description

Define a computation that calculates the eigenvalues of the gyration tensor and three shape parameters of multiple chunks of atoms. The computation includes all effects due to atoms passing through periodic boundaries.

The three computed shape parameters are the asphericity, b, the acylindricity, c, and the relative shape anisotropy, k:

$$
\begin{aligned}
c =& l_z - 0.5(l_y + l_x) \\
b =& l_y - l_x \\
k =& \frac{3}{2}\frac{l_x^2 + l_y^2 + l_z^2}{(l_x + l_y + l_z)^2} - \frac{1}{2}
\end{aligned}
$$

where l_x <= l_y <= :math`l_z` are the three eigenvalues of the gyration tensor. A general description of these parameters is provided in *(Mattice)* while an application to polymer systems can be found in *(Theodorou)*. The asphericity is always non-negative and zero only when the three principal moments are equal. This zero condition is met when the distribution of particles is spherically symmetric (hence the name asphericity) but also whenever the particle distribution is symmetric with respect to the three coordinate axes, e.g., when the particles are distributed uniformly on a cube, tetrahedron or other Platonic solid. The acylindricity is always non-negative and zero only when the two principal moments are equal. This zero condition is met when the distribution of particles is cylindrically symmetric (hence the name, acylindricity), but also whenever the particle distribution is symmetric with respect to the two coordinate axes, e.g., when the particles are distributed uniformly on a regular prism. the relative shape anisotropy is bounded between zero (if all points are spherically symmetric) and one (if all points lie on a line).

The tensor keyword must be specified in the compute gyration/chunk command.

Note: The coordinates of an atom contribute to the gyration tensor in "unwrapped" form, by using the image flags associated with each atom. See the *dump custom* command for a discussion of "unwrapped" coordinates. See the Atoms section of the *read_data* command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the *set image* command.

Output info:

This compute calculates a global array with six columns, which can be accessed by indices 1-6. The first three columns are the eigenvalues of the gyration tensor followed by the asphericity, the acylindricity and the relative shape anisotropy. The computed values can be used by any command that uses global array values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The array calculated by this compute is "intensive". The first five columns will be in distance^2 *units* while the sixth one is dimensionless.

17.43.4 Restrictions

This compute is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.43.5 Related commands

compute gyration/chunk compute gyration/shape

Default: none

(Mattice) Mattice, Suter, Conformational Theory of Large Molecules, Wiley, New York, 1994.

(Theodorou) Theodorou, Suter, Macromolecules, 18, 1206 (1985).

17.44 compute heat/flux command

17.44.1 Syntax

```
compute ID group-ID heat/flux ke-ID pe-ID stress-ID
```

- ID, group-ID are documented in *compute* command
- heat/flux = style name of this compute command
- ke-ID = ID of a compute that calculates per-atom kinetic energy
- pe-ID = ID of a compute that calculates per-atom potential energy
- stress-ID = ID of a compute that calculates per-atom stress

17.44.2 Examples

```
compute myFlux all heat/flux myKE myPE myStress
```

17.44.3 Description

Define a computation that calculates the heat flux vector based on contributions from atoms in the specified group. This can be used by itself to measure the heat flux through a set of atoms (e.g. a region between two thermostatted reservoirs held at different temperatures), or to calculate a thermal conductivity using the equilibrium Green-Kubo formalism.

For other non-equilibrium ways to compute a thermal conductivity, see the *Howto kappa* doc page.. These include use of the *fix thermal/conductivity* command for the Muller-Plathe method. Or the *fix heat* command which can add or subtract heat from groups of atoms.

The compute takes three arguments which are IDs of other *computes*. One calculates per-atom kinetic energy (*ke-ID*), one calculates per-atom potential energy (*pe-ID)*, and the third calculates per-atom stress (*stress-ID*).

Note: These other computes should provide values for all the atoms in the group this compute specifies. That means the other computes could use the same group as this compute, or they can just use group "all" (or any group whose atoms are superset of the atoms in this compute's group). LAMMPS does not check for this.

In case of two-body interactions, the heat flux is defined as:

$$
\begin{aligned}
\mathbf{J} &= \frac{1}{V}\left[\sum_i e_i \mathbf{v}_i - \sum_i \mathbf{S}_i \mathbf{v}_i\right] \\
&= \frac{1}{V}\left[\sum_i e_i \mathbf{v}_i + \sum_{i<j} \left(\mathbf{F}_{ij}\cdot\mathbf{v}_j\right)\mathbf{r}_{ij}\right] \\
&= \frac{1}{V}\left[\sum_i e_i \mathbf{v}_i + \frac{1}{2}\sum_{i<j} \left(\mathbf{F}_{ij}\cdot\left(\mathbf{v}_i+\mathbf{v}_j\right)\right)\mathbf{r}_{ij}\right]
\end{aligned}
$$

e_i in the first term of the equation is the per-atom energy (potential and kinetic). This is calculated by the computes *ke-ID* and *pe-ID*. $\mathbf{S}_i$ in the second term is the per-atom stress tensor calculated by the compute *stress-ID*. See *compute stress/atom* and *compute centroid/stress/atom* for possible definitions of atomic stress $\mathbf{S}_i$ in the case of bonded and many-body interactions. The tensor multiplies $\mathbf{v}_i$ as a 3x3 matrix-vector multiply to yield a vector. Note that as discussed below, the $1/V$ scaling factor in the equation for $\mathbf{J}$ is NOT included in the calculation performed by these computes; you need to add it for a volume appropriate to the atoms included in the calculation.

Note: The *compute pe/atom* and *compute stress/atom* commands have options for which terms to include in their calculation (pair, bond, etc). The heat flux calculation will thus include exactly the same terms. Normally you should use *compute stress/atom virial* or *compute centroid/stress/atom virial* so as not to include a kinetic energy term in the heat flux.

Warning: The compute *heat/flux* has been reported to produce unphysical values for angle, dihedral and improper contributions when used with *compute stress/atom*, as discussed in *(Surblys)* and *(Boone)*. You are strongly advised to use *compute centroid/stress/atom*, which has been implemented specifically for such cases.

The Green-Kubo formulas relate the ensemble average of the auto-correlation of the heat flux $\mathbf{J}$ to the thermal conductivity κ:

$$\kappa = \frac{V}{k_B T^2} \int_0^\infty \langle J_x(0) J_x(t) \rangle \, \mathrm{d}t = \frac{V}{3 k_B T^2} \int_0^\infty \langle \mathbf{J}(0) \cdot \mathbf{J}(t) \rangle \, \mathrm{d}t$$

The heat flux can be output every so many timesteps (e.g. via the *thermo_style custom* command). Then as a post-processing operation, an auto-correlation can be performed, its integral estimated, and the Green-Kubo formula above evaluated.

The *fix ave/correlate* command can calculate the auto-correlation. The trap() function in the *variable* command can calculate the integral.

An example LAMMPS input script for solid Ar is appended below. The result should be: average conductivity ~0.29 in W/mK.

Output info:

This compute calculates a global vector of length 6. The first 3 components are the x, y, z components of the full heat flux vector, i.e. (J_x, J_y, J_z). The next 3 components are the x, y, z components of just the convective portion of the flux, i.e. the first term in the equation for $\mathbf{J}$. Each component can be accessed by indices 1-6. These values can be used by any command that uses global vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector values calculated by this compute are "extensive", meaning they scale with the number of atoms in the simulation. They can be divided by the appropriate volume to get a flux, which would then be an "intensive" value, meaning independent of the number of atoms in the simulation. Note that if the compute is "all", then the appropriate volume to divide by is the simulation box volume. However, if a sub-group is used, it should be the volume containing those atoms.

The vector values will be in energy*velocity *units*. Once divided by a volume the units will be that of flux, namely energy/area/time *units*

17.44.4 Restrictions

none

17.44.5 Related commands

fix thermal/conductivity, *fix ave/correlate*, *variable*

Default: none

```
# Sample LAMMPS input script for thermal conductivity of solid Ar

units       real
variable    T equal 70
variable    V equal vol
variable    dt equal 4.0
variable    p equal 200     # correlation length
variable    s equal 10      # sample interval
```

```
variable    d equal $p*$s   # dump interval

# convert from LAMMPS real units to SI

variable    kB equal 1.3806504e-23    # [J/K] Boltzmann
variable    kCal2J equal 4186.0/6.02214e23
variable    A2m equal 1.0e-10
variable    fs2s equal 1.0e-15
variable    convert equal ${kCal2J}*${kCal2J}/${fs2s}/${A2m}

# setup problem

dimension    3
boundary     p p p
lattice      fcc 5.376 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1
region       box block 0 4 0 4 0 4
create_box   1 box
create_atoms 1 box
mass         1 39.948
pair_style   lj/cut 13.0
pair_coeff   * * 0.2381 3.405
timestep     ${dt}
thermo       $d

# equilibration and thermalization

velocity     all create $T 102486 mom yes rot yes dist gaussian
fix          NVT all nvt temp $T $T 10 drag 0.2
run          8000

# thermal conductivity calculation, switch to NVE if desired

#unfix       NVT
#fix         NVE all nve

reset_timestep 0
compute      myKE all ke/atom
compute      myPE all pe/atom
compute      myStress all stress/atom NULL virial
compute      flux all heat/flux myKE myPE myStress
variable     Jx equal c_flux[1]/vol
variable     Jy equal c_flux[2]/vol
variable     Jz equal c_flux[3]/vol
fix          JJ all ave/correlate $s $p $d &
             c_flux[1] c_flux[2] c_flux[3] type auto file J0Jt.dat ave running
variable     scale equal ${convert}/${kB}/$T/$T/$V*$s*${dt}
variable     k11 equal trap(f_JJ[3])*${scale}
variable     k22 equal trap(f_JJ[4])*${scale}
variable     k33 equal trap(f_JJ[5])*${scale}
thermo_style custom step temp v_Jx v_Jy v_Jz v_k11 v_k22 v_k33
run          100000
variable     k equal (v_k11+v_k22+v_k33)/3.0
variable     ndens equal count(all)/vol
print        "average conductivity: $k[W/mK] @ $T K, ${ndens} /A^3"
```

(Surblys) Surblys, Matsubara, Kikugawa, Ohara, Phys Rev E, 99, 051301(R) (2019).

(Boone) Boone, Babaei, Wilmer, J Chem Theory Comput, 15, 5579–5587 (2019).

17.45 compute hexorder/atom command

17.45.1 Syntax

```
compute ID group-ID hexorder/atom keyword values ...
```

- ID, group-ID are documented in *compute* command
- hexorder/atom = style name of this compute command
- one or more keyword/value pairs may be appended

```
keyword = degree or nnn or cutoff
  cutoff value = distance cutoff
  nnn value = number of nearest neighbors
  degree value = degree n of order parameter
```

17.45.2 Examples

```
compute 1 all hexorder/atom
compute 1 all hexorder/atom degree 4 nnn 4 cutoff 1.2
```

17.45.3 Description

Define a computation that calculates q_n the bond-orientational order parameter for each atom in a group. The hexatic (n = 6) order parameter was introduced by *Nelson and Halperin* as a way to detect hexagonal symmetry in two-dimensional systems. For each atom, q_n is a complex number (stored as two real numbers) defined as follows:

$$q_n = \frac{1}{nnn} \sum_{j=1}^{nnn} e^{ni\theta(\mathbf{r}_{ij})}$$

where the sum is over the *nnn* nearest neighbors of the central atom. The angle θ is formed by the bond vector r_{ij} and the x axis. θ is calculated only using the x and y components, whereas the distance from the central atom is calculated using all three x, y, and z components of the bond vector. Neighbor atoms not in the group are included in the order parameter of atoms in the group.

The optional keyword *cutoff* defines the distance cutoff used when searching for neighbors. The default value, also the maximum allowable value, is the cutoff specified by the pair style.

The optional keyword *nnn* defines the number of nearest neighbors used to calculate q_n. The default value is 6. If the value is NULL, then all neighbors up to the distance cutoff are used.

The optional keyword *degree* sets the degree n of the order parameter. The default value is 6. For a perfect hexagonal lattice with *nnn* = 6, $q_6 = e^{6i\phi}$ for all atoms, where the constant $0 < \phi < \frac{\pi}{3}$ depends only on the orientation of the lattice relative to the x axis. In an isotropic liquid, local neighborhoods may still exhibit weak hexagonal symmetry, but because the orientational correlation decays quickly with distance, the value of ϕ will be different for different atoms, and so when q_6 is averaged over all the atoms in the system, $|\langle q_6 \rangle| << 1$.

The value of q_n is set to zero for atoms not in the specified compute group, as well as for atoms that have less than *nnn* neighbors within the distance cutoff.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (i.e. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently.

Note: If you have a bonded system, then the settings of *special_bonds* command can remove pairwise interactions between atoms in the same bond, angle, or dihedral. This is the default setting for the *special_bonds* command, and means those pairwise interactions do not appear in the neighbor list. Because this fix uses the neighbor list, it also means those pairs will not be included in the order parameter. This difficulty can be circumvented by writing a dump file, and using the *rerun* command to compute the order parameter for snapshots in the dump file. The rerun script can use a *special_bonds* command that includes all pairs in the neighbor list.

Output info:

This compute calculates a per-atom array with 2 columns, giving the real and imaginary parts q_n, a complex number restricted to the unit disk of the complex plane i.e. $Re(q_n)^2 + Im(q_n)^2 <= 1$.

These values can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

17.45.4 Restrictions

none

17.45.5 Related commands

compute orientorder/atom, *compute coord/atom*, *compute centro/atom*

17.45.6 Default

The option defaults are *cutoff* = pair style cutoff, *nnn* = 6, *degree* = 6

(Nelson) Nelson, Halperin, Phys Rev B, 19, 2457 (1979).

17.46 compute hma command

17.46.1 Syntax

```
compute ID group-ID hma temp-ID keyword ...
```

- ID, group-ID are documented in *compute* command
- hma = style name of this compute command
- temp-ID = ID of fix that specifies the set temperature during canonical simulation
- keyword = *anharmonic u p Pharm cv*

```
anharmonic = compute will return anharmonic property values
u = compute will return potential energy
p = compute will return pressure.  the following keyword must be the␣
↪difference between the harmonic pressure and lattice pressure as described␣
↪below
cv = compute will return the heat capacity
```

17.46.2 Examples

```
compute 2 all hma 1 u
compute 2 all hma 1 anharmonic u p 0.9
compute 2 all hma 1 u cv
```

17.46.3 Description

Define a computation that calculates the properties of a solid (potential energy, pressure or heat capacity), using the harmonically-mapped averaging (HMA) method. This command yields much higher precision than the equivalent compute commands (*compute pe*, *compute pressure*, etc.) commands during a canonical simulation of an atomic crystal. Specifically, near melting HMA can yield averages of a given precision an order of magnitude faster than conventional methods, and this only improves as the temperatures is lowered. This is particularly important for evaluating the free energy by thermodynamic integration, where the low-temperature contributions are the greatest source of statistical uncertainty. Moreover, HMA has other advantages, including smaller potential-truncation effects, finite-size effects, smaller timestep inaccuracy, faster equilibration and shorter decorrelation time.

HMA should not be used if atoms are expected to diffuse. It is also restricted to simulations in the NVT ensemble. While this compute may be used with any potential in LAMMPS, it will provide inaccurate results for potentials that do not go to 0 at the truncation distance; *pair_style lj/smooth/linear* and Ewald summation should work fine, while *pair_style lj/cut* will perform poorly unless the potential is shifted (via *pair_modify* shift) or the cutoff is large. Furthermore, computation of the heat capacity with this compute is restricted to those that implement the *single_hessian* method in Pair. Implementing *single_hessian* in additional pair styles is simple. Please contact Andrew Schultz (ajs42 at buffalo.edu) and David Kofke (kofke at buffalo.edu) if your desired pair style does not have this method. This is the list of pair styles that currently implement *single_hessian*:

- *pair_style lj/smooth/linear*

In this method, the analytically known harmonic behavior of a crystal is removed from the traditional ensemble averages, which leads to an accurate and precise measurement of the anharmonic contributions without contamination by noise produced by the already-known harmonic behavior. A detailed description of this method can be found in (*Moustafa*). The potential energy is computed by the formula:

$$\langle U \rangle_{HMA} = \frac{d}{2}(N-1)k_B T + \left\langle U + \frac{1}{2} F \bullet \Delta r \right\rangle$$

where N is the number of atoms in the system, k_B is Boltzmann's constant, T is the temperature, d is the dimensionality of the system (2 or 3 for 2d/3d), $F \bullet \Delta r$ is the sum of dot products of the atomic force vectors and displacement (from lattice sites) vectors, and U is the sum of pair, bond, angle, dihedral, improper, kspace (long-range), and fix energies.

The pressure is computed by the formula:

$$\langle P \rangle_{HMA} = \Delta \hat{P} + \left\langle P_{vir} + \frac{\beta \Delta \hat{P} - \rho}{d(N-1)} F \bullet \Delta r \right\rangle$$

where ρ is the number density of the system, $\Delta \hat{P}$ is the difference between the harmonic and lattice pressure, P_{vir} is the virial pressure computed as the sum of pair, bond, angle, dihedral, improper, kspace (long-range), and fix

contributions to the force on each atom, and $k_B = 1/k_BT$. Although the method will work for any value of $\Delta\hat{P}$ specified (use pressure *units*), the precision of the resultant pressure is sensitive to $\Delta\hat{P}$; the precision tends to be best when $\Delta\hat{P}$ is the actual the difference between the lattice pressure and harmonic pressure.

$$\langle C_V \rangle_{HMA} = \frac{d}{2}(N-1)k_B + \frac{1}{k_BT^2}\left(\left\langle U_{HMA}^2 \right\rangle - \langle U_{HMA} \rangle^2\right) + \frac{1}{4T}\langle F \bullet \Delta r + \Delta r \bullet \Phi \bullet \Delta r \rangle$$

where Φ is the Hessian matrix. The compute hma command computes the full expression for C_V except for the $\left\langle U_{HMA}^2 \right\rangle^2$ in the variance term, which can be obtained by passing the *u* keyword; you must add this extra contribution to the C_V value reported by this compute. The variance term can cause significant round-off error when computing C_V. To address this, the *anharmonic* keyword can be passed and/or the output format can be specified with more digits.

```
thermo_modify format float '%22.15e'
```

The *anharmonic* keyword will instruct the compute to return anharmonic properties rather than the full properties, which include lattice, harmonic and anharmonic contributions. When using this keyword, the compute must be first active (it must be included via a *thermo_style custom* command) while the atoms are still at their lattice sites (before equilibration).

The temp-ID specified with compute hma command should be same as the fix-ID of Nose-Hoover (*fix nvt*) or Berendsen (*fix temp/berendsen*) thermostat used for the simulation. While using this command, Langevin thermostat (*fix langevin*) should be avoided as its extra forces interfere with the HMA implementation.

Note: Compute hma command should be used right after the energy minimization, when the atoms are at their lattice sites. The simulation should not be started before this command has been used in the input script.

The following example illustrates the placement of this command in the input script:

```
min_style cg
minimize 1e-35 1e-15 50000 500000
compute 1 all hma thermostatid u
fix thermostatid all nvt temp 600.0 600.0 100.0
```

Note: Compute hma should be used when the atoms of the solid do not diffuse. Diffusion will reduce the precision in the potential energy computation.

Note: The *fix_modify energy yes* command must also be specified if a fix is to contribute potential energy to this command.

An example input script that uses this compute is included in examples/USER/hma/ along with corresponding LAMMPS output showing that the HMA properties fluctuate less than the corresponding conventional properties.

Output info:

This compute calculates a global vector that includes the n properties requested as arguments to the command (the potential energy, pressure and/or heat capacity). The elements of the vector can be accessed by indices 1-n by any command that uses global vector values as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector values calculated by this compute are "extensive". The scalar value will be in energy *units*.

17.46.4 Restrictions

This compute is part of the USER-MISC package. It is enabled only if LAMMPS was built with that package. See the *Build package* doc page for more info.

Usage restricted to canonical (NVT) ensemble simulation only.

17.46.5 Related commands

compute pe, *compute pressure*

dynamical matrix provides a finite difference formulation of the hessian provided by Pair's single_hessian, which is used by this compute.

Default: none

(Moustafa) Sabry G. Moustafa, Andrew J. Schultz, and David A. Kofke, *Very fast averaging of thermal properties of crystals by molecular simulation*, Phys. Rev. E [92], 043303 (2015)

17.47 compute improper command

17.47.1 Syntax

```
compute ID group-ID improper
```

- ID, group-ID are documented in *compute* command
- improper = style name of this compute command

17.47.2 Examples

```
compute 1 all improper
```

17.47.3 Description

Define a computation that extracts the improper energy calculated by each of the improper sub-styles used in the *improper_style hybrid* command. These values are made accessible for output or further processing by other commands. The group specified for this command is ignored.

This compute is useful when using *improper_style hybrid* if you want to know the portion of the total energy contributed by one or more of the hybrid sub-styles.

Output info:

This compute calculates a global vector of length N where N is the number of sub_styles defined by the *improper_style hybrid* command. which can be accessed by indices 1-N. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector values are "extensive" and will be in energy *units*.

17.47.4 Restrictions

none

17.47.5 Related commands

compute pe, *compute pair*

Default: none

17.48 compute improper/local command

17.48.1 Syntax

```
compute ID group-ID improper/local value1 value2 ...
```

- ID, group-ID are documented in *compute* command
- improper/local = style name of this compute command
- one or more values may be appended
- value = *chi*

  chi = tabulate improper angles

17.48.2 Examples

```
compute 1 all improper/local chi
```

17.48.3 Description

Define a computation that calculates properties of individual improper interactions. The number of datums generated, aggregated across all processors, equals the number of impropers in the system, modified by the group parameter as explained below.

The value *chi* is the improper angle, as defined in the doc pages for the individual improper styles listed on *improper_style* doc page.

The local data stored by this command is generated by looping over all the atoms owned on a processor and their impropers. An improper will only be included if all 4 atoms in the improper are in the specified compute group.

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For example, improper output from the *compute property/local* command can be combined with data from this command and output by the *dump local* command in a consistent way.

Here is an example of how to do this:

```
compute 1 all property/local itype iatom1 iatom2 iatom3 iatom4
compute 2 all improper/local chi
dump 1 all local 1000 tmp.dump index c_1[1] c_1[2] c_1[3] c_1[4] c_1[5] c_2[1]
```

Output info:

This compute calculates a local vector or local array depending on the number of keywords. The length of the vector or number of rows in the array is the number of impropers. If a single keyword is specified, a local vector is produced. If two or more keywords are specified, a local array is produced where the number of columns = the number of keywords. The vector or array can be accessed by any command that uses local values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The output for *chi* will be in degrees.

17.48.4 Restrictions

none

17.48.5 Related commands

dump local, *compute property/local*

Default: none

17.49 compute inertia/chunk command

17.49.1 Syntax

```
compute ID group-ID inertia/chunk chunkID
```

- ID, group-ID are documented in *compute* command
- inertia/chunk = style name of this compute command
- chunkID = ID of *compute chunk/atom* command

17.49.2 Examples

```
compute 1 fluid inertia/chunk molchunk
```

17.49.3 Description

Define a computation that calculates the inertia tensor for multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a *compute chunk/atom* command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the *compute chunk/atom* and *Howto chunk* doc pages for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

This compute calculates the 6 components of the symmetric inertia tensor for each chunk, ordered Ixx,Iyy,Izz,Ixy,Iyz,Ixz. The calculation includes all effects due to atoms passing through periodic boundaries.

Note that only atoms in the specified group contribute to the calculation. The *compute chunk/atom* command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

Note: The coordinates of an atom contribute to the chunk's inertia tensor in "unwrapped" form, by using the image flags associated with each atom. See the *dump custom* command for a discussion of "unwrapped" coordinates. See the Atoms section of the *read_data* command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the *set image* command.

The simplest way to output the results of the compute inertia/chunk calculation to a file is to use the *fix ave/time* command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all inertia/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk[*] file tmp.out mode vector
```

Output info:

This compute calculates a global array where the number of rows = the number of chunks *Nchunk* as calculated by the specified *compute chunk/atom* command. The number of columns = 6 for the 6 components of the inertia tensor for each chunk, ordered as listed above. These values can be accessed by any command that uses global array values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The array values are "intensive". The array values will be in mass*distance^2 *units*.

17.49.4 Restrictions

none

17.49.5 Related commands

variable inertia() function

Default: none

17.50 compute ke command

17.50.1 Syntax

```
compute ID group-ID ke
```

- ID, group-ID are documented in *compute* command
- ke = style name of this compute command

17.50.2 Examples

```
compute 1 all ke
```

17.50.3 Description

Define a computation that calculates the translational kinetic energy of a group of particles.

The kinetic energy of each particle is computed as $\frac{1}{2}mv^2$, where *m* and *v* are the mass and velocity of the particle.

There is a subtle difference between the quantity calculated by this compute and the kinetic energy calculated by the *ke* or *etotal* keyword used in thermodynamic output, as specified by the *thermo_style* command. For this compute, kinetic energy is "translational" kinetic energy, calculated by the simple formula above. For thermodynamic output, the *ke* keyword infers kinetic energy from the temperature of the system with $\frac{1}{2}k_BT$ of energy for each degree of freedom. For the default temperature computation via the *compute temp* command, these are the same. But different computes that calculate temperature can subtract out different non-thermal components of velocity and/or include different degrees of freedom (translational, rotational, etc).

Output info:

This compute calculates a global scalar (the summed KE). This value can be used by any command that uses a global scalar value from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy *units*.

17.50.4 Restrictions

none

17.50.5 Related commands

compute erotate/sphere

Default: none

17.51 compute ke/atom command

17.51.1 Syntax

```
compute ID group-ID ke/atom
```

- ID, group-ID are documented in *compute* command
- ke/atom = style name of this compute command

17.51.2 Examples

```
compute 1 all ke/atom
```

17.51.3 Description

Define a computation that calculates the per-atom translational kinetic energy for each atom in a group.

The kinetic energy is simply 1/2 m v^2, where m is the mass and v is the velocity of each atom.

The value of the kinetic energy will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values will be in energy *units*.

17.51.4 Restrictions

none

17.51.5 Related commands

dump custom

Default: none

17.52 compute ke/atom/eff command

17.52.1 Syntax

```
compute ID group-ID ke/atom/eff
```

- ID, group-ID are documented in *compute* command
- ke/atom/eff = style name of this compute command

17.52.2 Examples

```
compute 1 all ke/atom/eff
```

17.52.3 Description

Define a computation that calculates the per-atom translational (nuclei and electrons) and radial kinetic energy (electron only) in a group. The particles are assumed to be nuclei and electrons modeled with the *electronic force field*.

The kinetic energy for each nucleus is computed as $\frac{1}{2}mv^2$, where *m* corresponds to the corresponding nuclear mass, and the kinetic energy for each electron is computed as $\frac{1}{2}(m_e v^2 + \frac{3}{4}m_e s^2)$, where m_e and *v* correspond to the mass and translational velocity of each electron, and *s* to its radial velocity, respectively.

There is a subtle difference between the quantity calculated by this compute and the kinetic energy calculated by the *ke* or *etotal* keyword used in thermodynamic output, as specified by the *thermo_style* command. For this compute, kinetic energy is "translational" plus electronic "radial" kinetic energy, calculated by the simple formula above. For

thermodynamic output, the *ke* keyword infers kinetic energy from the temperature of the system with $\frac{1}{2}k_BT$ of energy for each (nuclear-only) degree of freedom in eFF.

Note: The temperature in eFF should be monitored via the *compute temp/eff* command, which can be printed with thermodynamic output by using the *thermo_modify* command, as shown in the following example:

```
compute         effTemp all temp/eff
thermo_style    custom step etotal pe ke temp press
thermo_modify   temp effTemp
```

The value of the kinetic energy will be 0.0 for atoms (nuclei or electrons) not in the specified compute group.

Output info:

This compute calculates a scalar quantity for each atom, which can be accessed by any command that uses per-atom computes as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values will be in energy *units*.

17.52.4 Restrictions

This compute is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.52.5 Related commands

dump custom

Default: none

17.53 compute ke/eff command

17.53.1 Syntax

```
compute ID group-ID ke/eff
```

- ID, group-ID are documented in *compute* command
- ke/eff = style name of this compute command

17.53.2 Examples

```
compute 1 all ke/eff
```

17.53.3 Description

Define a computation that calculates the kinetic energy of motion of a group of eFF particles (nuclei and electrons), as modeled with the *electronic force field*.

The kinetic energy for each nucleus is computed as $\frac{1}{2}mv^2$ and the kinetic energy for each electron is computed as $\frac{1}{2}(m_e v^2 + \frac{3}{4}m_e s^2)$, where *m* corresponds to the nuclear mass, m_e to the electron mass, *v* to the translational velocity of each particle, and *s* to the radial velocity of the electron, respectively.

There is a subtle difference between the quantity calculated by this compute and the kinetic energy calculated by the *ke* or *etotal* keyword used in thermodynamic output, as specified by the *thermo_style* command. For this compute, kinetic energy is "translational" and "radial" (only for electrons) kinetic energy, calculated by the simple formula above. For thermodynamic output, the *ke* keyword infers kinetic energy from the temperature of the system with $\frac{1}{2}k_B T$ of energy for each degree of freedom. For the eFF temperature computation via the *compute temp_eff* command, these are the same. But different computes that calculate temperature can subtract out different non-thermal components of velocity and/or include other degrees of freedom.

Warning: The temperature in eFF models should be monitored via the *compute temp/eff* command, which can be printed with thermodynamic output by using the *thermo_modify* command, as shown in the following example:

```
compute         effTemp all temp/eff
thermo_style    custom step etotal pe ke temp press
thermo_modify   temp effTemp
```

See *compute temp/eff*.

Output info:

This compute calculates a global scalar (the KE). This value can be used by any command that uses a global scalar value from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy *units*.

17.53.4 Restrictions

This compute is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Related commands: none

Default: none

17.54 compute ke/rigid command

17.54.1 Syntax

```
compute ID group-ID ke/rigid fix-ID
```

- ID, group-ID are documented in *compute* command
- ke = style name of this compute command
- fix-ID = ID of rigid body fix

17.54.2 Examples

```
compute 1 all ke/rigid myRigid
```

17.54.3 Description

Define a computation that calculates the translational kinetic energy of a collection of rigid bodies, as defined by one of the *fix rigid* command variants.

The kinetic energy of each rigid body is computed as 1/2 M Vcm^2, where M is the total mass of the rigid body, and Vcm is its center-of-mass velocity.

The *fix-ID* should be the ID of one of the *fix rigid* commands which defines the rigid bodies. The group specified in the compute command is ignored. The kinetic energy of all the rigid bodies defined by the fix rigid command in included in the calculation.

Output info:

This compute calculates a global scalar (the summed KE of all the rigid bodies). This value can be used by any command that uses a global scalar value from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy *units*.

17.54.4 Restrictions

This compute is part of the RIGID package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.54.5 Related commands

compute erotate/rigid

Default: none

17.55 compute meso/e/atom command

17.55.1 Syntax

```
compute ID group-ID meso/e/atom
```

- ID, group-ID are documented in *compute* command
- meso/e/atom = style name of this compute command

17.55.2 Examples

```
compute 1 all meso/e/atom
```

17.55.3 Description

Define a computation that calculates the per-atom internal energy for each atom in a group.

The internal energy is the energy associated with the internal degrees of freedom of a mesoscopic particles, e.g. a Smooth-Particle Hydrodynamics particle.

See this PDF guide to using SPH in LAMMPS.

The value of the internal energy will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values will be in energy *units*.

17.55.4 Restrictions

This compute is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.55.5 Related commands

dump custom

Default: none

17.56 compute meso/rho/atom command

17.56.1 Syntax

```
compute ID group-ID meso/rho/atom
```

- ID, group-ID are documented in *compute* command
- meso/rho/atom = style name of this compute command

17.56.2 Examples

```
compute 1 all meso/rho/atom
```

17.56.3 Description

Define a computation that calculates the per-atom mesoscopic density for each atom in a group.

The mesoscopic density is the mass density of a mesoscopic particle, calculated by kernel function interpolation using "pair style sph/rhosum".

See this PDF guide to using SPH in LAMMPS.

The value of the mesoscopic density will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values will be in mass/volume *units*.

17.56.4 Restrictions

This compute is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.56.5 Related commands

dump custom

Default: none

17.57 compute meso/t/atom command

17.57.1 Syntax

```
compute ID group-ID meso/t/atom
```

- ID, group-ID are documented in *compute* command
- meso/t/atom = style name of this compute command

17.57.2 Examples

```
compute 1 all meso/t/atom
```

17.57.3 Description

Define a computation that calculates the per-atom internal temperature for each atom in a group.

The internal temperature is the ratio of internal energy over the heat capacity associated with the internal degrees of freedom of a mesoscopic particles, e.g. a Smooth-Particle Hydrodynamics particle.

T_*int* = E_*int* / C_*V, int*

See this PDF guide to using SPH in LAMMPS.

The value of the internal energy will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values will be in temperature *units*.

17.57.4 Restrictions

This compute is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.57.5 Related commands

dump custom

Default: none

17.58 compute momentum command

17.58.1 Syntax

```
compute ID group-ID momentum
```

- ID, group-ID are documented in *compute* command
- momentum = style name of this compute command

17.58.2 Examples

```
compute 1 all momentum
```

17.58.3 Description

Define a computation that calculates the translational momentum of a group of particles.

The momentum of each particles is computed as m v, where m and v are the mass and velocity of the particle.

Output info:

This compute calculates a global vector (the summed momentum) of length 3. This value can be used by any command that uses a global vector value from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector value calculated by this compute is "extensive". The vector value will be in mass*velocity *units*.

17.58.4 Restrictions

This compute is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.58.5 Related commands

Default: none

17.59 compute msd command

17.59.1 Syntax

```
compute ID group-ID msd keyword values ...
```

- ID, group-ID are documented in *compute* command
- msd = style name of this compute command
- zero or more keyword/value pairs may be appended
- keyword = *com* or *average*

  com value = *yes* or *no*
  average value = *yes* or *no*

17.59.2 Examples

```
compute 1 all msd
compute 1 upper msd com yes average yes
```

17.59.3 Description

Define a computation that calculates the mean-squared displacement (MSD) of the group of atoms, including all effects due to atoms passing through periodic boundaries. For computation of the non-Gaussian parameter of mean-squared displacement, see the *compute msd/nongauss* command.

A vector of four quantities is calculated by this compute. The first 3 elements of the vector are the squared dx,dy,dz displacements, summed and averaged over atoms in the group. The 4th element is the total squared displacement, i.e. (dx*dx + dy*dy + dz*dz), summed and averaged over atoms in the group.

The slope of the mean-squared displacement (MSD) versus time is proportional to the diffusion coefficient of the diffusing atoms.

The displacement of an atom is from its reference position. This is normally the original position at the time the compute command was issued, unless the *average* keyword is set to *yes*. The value of the displacement will be 0.0 for atoms not in the specified compute group.

If the *com* option is set to *yes* then the effect of any drift in the center-of-mass of the group of atoms is subtracted out before the displacement of each atom is calculated.

If the *average* option is set to *yes* then the reference position of an atom is based on the average position of that atom, corrected for center-of-mass motion if requested. The average position is a running average over all previous calls to the compute, including the current call. So on the first call it is current position, on the second call it is the arithmetic average of the current position and the position on the first call, and so on. Note that when using this option, the precise value of the mean square displacement will depend on the number of times the compute is called. So, for example, changing the frequency of thermo output may change the computed displacement. Also, the precise values will be changed if a single simulation is broken up into two parts, using either multiple run commands or a restart file. It only makes sense to use this option if the atoms are not diffusing, so that their average positions relative to the center of mass of the system are stationary. The most common case is crystalline solids undergoing thermal motion.

Note: Initial coordinates are stored in "unwrapped" form, by using the image flags associated with each atom. See the *dump custom* command for a discussion of "unwrapped" coordinates. See the Atoms section of the *read_data* command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the *set image* command.

Note: If you want the quantities calculated by this compute to be continuous when running from a *restart file*, then you should use the same ID for this compute, as in the original run. This is so that the fix this compute creates to store per-atom quantities will also have the same ID, and thus be initialized correctly with atom reference positions from the restart file. When *average* is set to yes, then the atom reference positions are restored correctly, but not the number of samples used obtain them. As a result, the reference positions from the restart file are combined with subsequent positions as if they were from a single sample, instead of many, which will change the values of msd somewhat.

Output info:

This compute calculates a global vector of length 4, which can be accessed by indices 1-4 by any command that uses global vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector values are "intensive". The vector values will be in distance^2 *units*.

17.59.4 Restrictions

none

17.59.5 Related commands

compute msd/nongauss, *compute displace_atom*, *fix store/state*, *compute msd/chunk*

17.59.6 Default

The option default are com = no, average = no.

17.60 compute msd/chunk command

17.60.1 Syntax

```
compute ID group-ID msd/chunk chunkID
```

- ID, group-ID are documented in *compute* command
- msd/chunk = style name of this compute command
- chunkID = ID of *compute chunk/atom* command

17.60.2 Examples

```
compute 1 all msd/chunk molchunk
```

17.60.3 Description

Define a computation that calculates the mean-squared displacement (MSD) for multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a *compute chunk/atom* command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the *compute chunk/atom* and *Howto chunk* doc pages for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

Four quantities are calculated by this compute for each chunk. The first 3 quantities are the squared dx,dy,dz displacements of the center-of-mass. The 4th component is the total squared displacement, i.e. (dx*dx + dy*dy + dz*dz) of the center-of-mass. These calculations include all effects due to atoms passing through periodic boundaries.

Note that only atoms in the specified group contribute to the calculation. The *compute chunk/atom* command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

The slope of the mean-squared displacement (MSD) versus time is proportional to the diffusion coefficient of the diffusing chunks.

The displacement of the center-of-mass of the chunk is from its original center-of-mass position, calculated on the timestep this compute command was first invoked.

Note: The number of chunks *Nchunk* calculated by the *compute chunk/atom* command must remain constant each time this compute is invoked, so that the displacement for each chunk from its original position can be computed consistently. If *Nchunk* does not remain constant, an error will be generated. If needed, you can enforce a constant *Nchunk* by using the *nchunk once* or *ids once* options when specifying the *compute chunk/atom* command.

Note: This compute stores the original position (of the center-of-mass) of each chunk. When a displacement is calculated on a later timestep, it is assumed that the same atoms are assigned to the same chunk ID. However LAMMPS has no simple way to insure this is the case, though you can use the *ids once* option when specifying the *compute chunk/atom* command. Note that if this is not the case, the MSD calculation does not have a sensible meaning.

Note: The initial coordinates of the atoms in each chunk are stored in "unwrapped" form, by using the image flags associated with each atom. See the *dump custom* command for a discussion of "unwrapped" coordinates. See the Atoms section of the *read_data* command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the *set image* command.

Note: If you want the quantities calculated by this compute to be continuous when running from a *restart file*, then you should use the same ID for this compute, as in the original run. This is so that the fix this compute creates to store per-chunk quantities will also have the same ID, and thus be initialized correctly with chunk reference positions from the restart file.

The simplest way to output the results of the compute msd/chunk calculation to a file is to use the *fix ave/time* command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all msd/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk[*] file tmp.out mode vector
```

Output info:

This compute calculates a global array where the number of rows = the number of chunks *Nchunk* as calculated by the specified *compute chunk/atom* command. The number of columns = 4 for dx,dy,dz and the total displacement. These values can be accessed by any command that uses global array values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The array values are "intensive". The array values will be in distance^2 *units*.

17.60.4 Restrictions

none

17.60.5 Related commands

compute msd

Default: none

17.61 compute msd/nongauss command

17.61.1 Syntax

```
compute ID group-ID msd/nongauss keyword values ...
```

- ID, group-ID are documented in *compute* command
- msd/nongauss = style name of this compute command
- zero or more keyword/value pairs may be appended
- keyword = *com*

  com value = *yes* or *no*

17.61.2 Examples

```
compute 1 all msd/nongauss
compute 1 upper msd/nongauss com yes
```

17.61.3 Description

Define a computation that calculates the mean-squared displacement (MSD) and non-Gaussian parameter (NGP) of the group of atoms, including all effects due to atoms passing through periodic boundaries.

A vector of three quantities is calculated by this compute. The first element of the vector is the total squared dx,dy,dz displacements drsquared = (dx*dx + dy*dy + dz*dz) of atoms, and the second is the fourth power of these displacements drfourth = (dx*dx + dy*dy + dz*dz)*(dx*dx + dy*dy + dz*dz), summed and averaged over atoms in the group. The 3rd component is the nonGaussian diffusion parameter NGP = 3*drfourth/(5*drsquared*drsquared), i.e.

$$NGP(t) = 3 < (r(t) - r(0))^4 > /(5 < (r(t) - r(0))^2 >^2) - 1$$

The NGP is a commonly used quantity in studies of dynamical heterogeneity. Its minimum theoretical value (-0.4) occurs when all atoms have the same displacement magnitude. NGP=0 for Brownian diffusion, while NGP > 0 when some mobile atoms move faster than others.

If the *com* option is set to *yes* then the effect of any drift in the center-of-mass of the group of atoms is subtracted out before the displacement of each atom is calculated.

See the *compute msd* doc page for further important NOTEs, which also apply to this compute.

Output info:

This compute calculates a global vector of length 3, which can be accessed by indices 1-3 by any command that uses global vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector values are "intensive". The first vector value will be in distance^2 *units*, the second is in distance^4 units, and the 3rd is dimensionless.

17.61.4 Restrictions

This compute is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.61.5 Related commands

compute msd

17.61.6 Default

The option default is com = no.

17.62 compute omega/chunk command

17.62.1 Syntax

```
compute ID group-ID omega/chunk chunkID
```

- ID, group-ID are documented in *compute* command
- omega/chunk = style name of this compute command
- chunkID = ID of *compute chunk/atom* command

17.62.2 Examples

```
compute 1 fluid omega/chunk molchunk
```

17.62.3 Description

Define a computation that calculates the angular velocity (omega) of multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a *compute chunk/atom* command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the *compute chunk/atom* and *Howto chunk* doc pages for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

This compute calculates the 3 components of the angular velocity vector for each chunk, via the formula L = Iw where L is the angular momentum vector of the chunk, I is its moment of inertia tensor, and w is omega = angular velocity of the chunk. The calculation includes all effects due to atoms passing through periodic boundaries.

Note that only atoms in the specified group contribute to the calculation. The *compute chunk/atom* command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

Note: The coordinates of an atom contribute to the chunk's angular velocity in "unwrapped" form, by using the image flags associated with each atom. See the *dump custom* command for a discussion of "unwrapped" coordinates. See

the Atoms section of the *read_data* command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the *set image* command.

The simplest way to output the results of the compute omega/chunk calculation to a file is to use the *fix ave/time* command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all omega/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk[*] file tmp.out mode vector
```

Output info:

This compute calculates a global array where the number of rows = the number of chunks *Nchunk* as calculated by the specified *compute chunk/atom* command. The number of columns = 3 for the 3 xyz components of the angular velocity for each chunk. These values can be accessed by any command that uses global array values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The array values are "intensive". The array values will be in velocity/distance *units*.

17.62.4 Restrictions

none

17.62.5 Related commands

variable omega() function

Default: none

17.63 compute orientorder/atom command

17.63.1 Syntax

```
compute ID group-ID orientorder/atom keyword values ...
```

- ID, group-ID are documented in *compute* command
- orientorder/atom = style name of this compute command
- one or more keyword/value pairs may be appended

```
keyword = cutoff or nnn or degrees or components
  cutoff value = distance cutoff
  nnn value = number of nearest neighbors
  degrees values = nlvalues, l1, l2,...
  wl value = yes or no
  wl/hat value = yes or no
  components value = ldegree
```

17.63.2 Examples

```
compute 1 all orientorder/atom
compute 1 all orientorder/atom degrees 5 4 6 8 10 12 nnn NULL cutoff 1.5
compute 1 all orientorder/atom wl/hat yes
compute 1 all orientorder/atom components 6
```

17.63.3 Description

Define a computation that calculates a set of bond-orientational order parameters Q_l for each atom in a group. These order parameters were introduced by *Steinhardt et al.* as a way to characterize the local orientational order in atomic structures. For each atom, Q_l is a real number defined as follows:

$$\bar{Y}_{lm} = \frac{1}{nnn} \sum_{j=1}^{nnn} Y_{lm}(\theta(\mathbf{r}_{ij}), \phi(\mathbf{r}_{ij}))$$

$$Q_l = \sqrt{\frac{4\pi}{2l+1} \sum_{m=-l}^{m=l} \bar{Y}_{lm} \bar{Y}^*_{lm}}$$

The first equation defines the spherical harmonic order parameters. These are complex number components of the 3D analog of the 2D order parameter q_n, which is implemented as LAMMPS compute *hexorder/atom*. The summation is over the *nnn* nearest neighbors of the central atom. The angles theta and phi are the standard spherical polar angles defining the direction of the bond vector r_{ij}. The second equation defines Q_l, which is a rotationally invariant non-negative amplitude obtained by summing over all the components of degree *l*.

The optional keyword *cutoff* defines the distance cutoff used when searching for neighbors. The default value, also the maximum allowable value, is the cutoff specified by the pair style.

The optional keyword *nnn* defines the number of nearest neighbors used to calculate Q_l. The default value is 12. If the value is NULL, then all neighbors up to the specified distance cutoff are used.

The optional keyword *degrees* defines the list of order parameters to be computed. The first argument *nlvalues* is the number of order parameters. This is followed by that number of non-negative integers giving the degree of each order parameter. Because Q_2 and all odd-degree order parameters are zero for atoms in cubic crystals (see *Steinhardt*), the default order parameters are Q_4, Q_6, Q_8, Q_{10}, and Q_{12}. For the FCC crystal with *nnn* =12, $Q_4 = \sqrt{\frac{7}{192}} = 0.19094....$ The numerical values of all order parameters up to Q_12 for a range of commonly encountered high-symmetry structures are given in Table I of *Mickel et al.*, and these can be reproduced with this compute.

The optional keyword *wl* will output the third-order invariants W_l (see Eq. 1.4 in *Steinhardt*) for the same degrees as for the Q_l parameters. For the FCC crystal with *nnn* =12, W_4 = -sqrt(14/143).(49/4096)/Pi^1.5 = -0.0006722136...

The optional keyword *wl/hat* will output the normalized third-order invariants $\hat{W}_l$ (see Eq. 2.2 in *Steinhardt*) for the same degrees as for the Q_l parameters. For the FCC crystal with *nnn* =12, $\hat{W}_4 = -\frac{7}{3}\sqrt{\frac{2}{429}} = -0.159317...$ The numerical values of $\hat{W}_l$ for a range of commonly encountered high-symmetry structures are given in Table I of *Steinhardt*, and these can be reproduced with this keyword.

The optional keyword *components* will output the components of the normalized complex vector $\bar{Y}_{lm}$ of degree *ldegree*, which must be explicitly included in the keyword *degrees*. This option can be used in conjunction with *compute coord_atom* to calculate the ten Wolde's criterion to identify crystal-like particles, as discussed in *ten Wolde*.

The value of Q_l is set to zero for atoms not in the specified compute group, as well as for atoms that have less than *nnn* neighbors within the distance cutoff, unless *nnn* is NULL.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (i.e. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently.

Note: If you have a bonded system, then the settings of *special_bonds* command can remove pairwise interactions between atoms in the same bond, angle, or dihedral. This is the default setting for the *special_bonds* command, and means those pairwise interactions do not appear in the neighbor list. Because this fix uses the neighbor list, it also means those pairs will not be included in the order parameter. This difficulty can be circumvented by writing a dump file, and using the *rerun* command to compute the order parameter for snapshots in the dump file. The rerun script can use a *special_bonds* command that includes all pairs in the neighbor list.

Output info:

This compute calculates a per-atom array with *nlvalues* columns, giving the Q_l values for each atom, which are real numbers on the range $0 <= Q_l <= 1$.

If the keyword *wl* is set to yes, then the W_l values for each atom will be added to the output array, which are real numbers.

If the keyword *wl/hat* is set to yes, then the $\hat{W}_l$ values for each atom will be added to the output array, which are real numbers.

If the keyword *components* is set, then the real and imaginary parts of each component of (normalized) $\bar{Y}_{lm}$ will be added to the output array in the following order: $Re(\bar{Y}_{-m})Im(\bar{Y}_{-m})Re(\bar{Y}_{-m+1})Im(\bar{Y}_{-m+1})...Re(\bar{Y}_m)Im(\bar{Y}_m)$. This way, the per-atom array will have a total of *nlvalues*+2*(2*l*+1) columns.

These values can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

17.63.4 Restrictions

none

17.63.5 Related commands

compute coord/atom, *compute centro/atom*, *compute hexorder/atom*

17.63.6 Default

The option defaults are *cutoff* = pair style cutoff, *nnn* = 12, *degrees* = 5 4 6 8 10 12 i.e. Q_4, Q_6, Q_8, Q_{10}, and Q_{12}, *wl* = no, *wl/hat* = no, and *components* off

(Steinhardt) P. Steinhardt, D. Nelson, and M. Ronchetti, Phys. Rev. B 28, 784 (1983).

(Mickel) W. Mickel, S. C. Kapfer, G. E. Schroeder-Turkand, K. Mecke, J. Chem. Phys. 138, 044501 (2013).

(tenWolde) P. R. ten Wolde, M. J. Ruiz-Montero, D. Frenkel, J. Chem. Phys. 104, 9932 (1996).

17.64 compute pair command

17.64.1 Syntax

```
compute ID group-ID pair pstyle [nstyle] [evalue]
```

- ID, group-ID are documented in *compute* command
- pair = style name of this compute command
- pstyle = style name of a pair style that calculates additional values
- nsub = *n*-instance of a sub-style, if a pair style is used multiple times in a hybrid style
- *evalue* = *epair* or *evdwl* or *ecoul* or blank (optional)

17.64.2 Examples

```
compute 1 all pair gauss
compute 1 all pair lj/cut/coul/cut ecoul
compute 1 all pair tersoff 2 epair
compute 1 all pair reax/c
```

17.64.3 Description

Define a computation that extracts additional values calculated by a pair style, and makes them accessible for output or further processing by other commands.

Note: The group specified for this command is **ignored**.

The specified *pstyle* must be a pair style used in your simulation either by itself or as a sub-style in a *pair_style hybrid or hybrid/overlay* command. If the sub-style is used more than once, an additional number *nsub* has to be specified in order to choose which instance of the sub-style will be used by the compute. Not specifying the number in this case will cause the compute to fail.

The *evalue* setting is optional. All pair styles tally a potential energy *epair* which may be broken into two parts: *evdwl* and *ecoul* such that *epair* = *evdwl* + *ecoul*. If the pair style calculates Coulombic interactions, their energy will be tallied in *ecoul*. Everything else (whether it is a Lennard-Jones style van der Waals interaction or not) is tallied in *evdwl*. If *evalue* is blank or specified as *epair*, then *epair* is stored as a global scalar by this compute. This is useful when using *pair_style hybrid* if you want to know the portion of the total energy contributed by one sub-style. If *evalue* is specified as *evdwl* or *ecoul*, then just that portion of the energy is stored as a global scalar.

Note: The energy returned by the *evdwl* keyword does not include tail corrections, even if they are enabled via the *pair_modify* command.

Some pair styles tally additional quantities, e.g. a breakdown of potential energy into 14 components is tallied by the *pair_style reax/c* command. These values (1 or more) are stored as a global vector by this compute. See the doc page for *individual pair styles* for info on these values.

Output info:

This compute calculates a global scalar which is *epair* or *evdwl* or *ecoul*. If the pair style supports it, it also calculates a global vector of length >= 1, as determined by the pair style. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar and vector values calculated by this compute are "extensive".

The scalar value will be in energy *units*. The vector values will typically also be in energy *units*, but see the doc page for the pair style for details.

17.64.4 Restrictions

none

17.64.5 Related commands

compute pe, *compute bond*

17.64.6 Default

The keyword defaults are *evalue* = *epair*, nsub = 0.

17.65 compute pair/local command

17.65.1 Syntax

```
compute ID group-ID pair/local value1 value2 ... keyword args ...
```

- ID, group-ID are documented in *compute* command
- pair/local = style name of this compute command
- one or more values may be appended
- value = *dist* or *eng* or *force* or *fx* or *fy* or *fz* or *pN*

  ```
  dist = pairwise distance
  eng = pairwise energy
  force = pairwise force
  fx,fy,fz = components of pairwise force
  pN = pair style specific quantities for allowed N values
  ```

- zero or more keyword/arg pairs may be appended
- keyword = *cutoff*

  ```
  cutoff arg = type or radius
  ```

17.65.2 Examples

```
compute 1 all pair/local eng
compute 1 all pair/local dist eng force
compute 1 all pair/local dist eng fx fy fz
compute 1 all pair/local dist fx fy fz p1 p2 p3
```

17.65.3 Description

Define a computation that calculates properties of individual pairwise interactions. The number of datums generated, aggregated across all processors, equals the number of pairwise interactions in the system.

The local data stored by this command is generated by looping over the pairwise neighbor list. Info about an individual pairwise interaction will only be included if both atoms in the pair are in the specified compute group, and if the current pairwise distance is less than the force cutoff distance for that interaction, as defined by the *pair_style* and *pair_coeff* commands.

The value *dist* is the distance between the pair of atoms.

The value *eng* is the interaction energy for the pair of atoms.

The value *force* is the force acting between the pair of atoms, which is positive for a repulsive force and negative for an attractive force. The values *fx*, *fy*, and *fz* are the xyz components of *force* on atom I.

A pair style may define additional pairwise quantities which can be accessed as *p1* to *pN*, where N is defined by the pair style. Most pair styles do not define any additional quantities, so N = 0. An example of ones that do are the *granular pair styles* which calculate the tangential force between two particles and return its components and magnitude acting on atom I for N = 1,2,3,4. See individual pair styles for details.

When using *pN* with pair style *hybrid*, the output will be the Nth quantity from the sub-style that computes the pairwise interaction (based on atom types). If that sub-style does not define a *pN*, the output will be 0.0. The maximum allowed N is the maximum number of quantities provided by any sub-style.

When using *pN* with pair style *hybrid/overlay* the quantities from all sub-styles that provide them are concatenated together into one long list. For example, if there are 3 sub-styles and 2 of them have additional output (with 3 and 4 quantities, respectively), then 7 values (*p1* up to *p7*) are defined. The values *p1* to *p3* refer to quantities defined by the first of the two sub-styles. Values *p4* to *p7* refer to quantities from the second of the two sub-styles. If the referenced *pN* is not computed for the specific pairwise interaction (based on atom types), then the output will be 0.0.

The value *dist* will be in distance *units*. The value *eng* will be in energy *units*. The values *force*, *fx*, *fy*, and *fz* will be in force *units*. The values *pN* will be in whatever units the pair style defines.

The optional *cutoff* keyword determines how the force cutoff distance for an interaction is determined. For the default setting of *type*, the pairwise cutoff defined by the *pair_style* command for the types of the two atoms is used. For the *radius* setting, the sum of the radii of the two particles is used as a cutoff. For example, this is appropriate for granular particles which only interact when they are overlapping, as computed by *granular pair styles*. Note that if a granular model defines atom types such that all particles of a specific type are monodisperse (same diameter), then the two settings are effectively identical.

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For example, pair output from the *compute property/local* command can be combined with data from this command and output by the *dump local* command in a consistent way.

Here is an example of how to do this:

```
compute 1 all property/local patom1 patom2
compute 2 all pair/local dist eng force
dump 1 all local 1000 tmp.dump index c_1[1] c_1[2] c_2[1] c_2[2] c_2[3]
```

Note: For pairs, if two atoms I,J are involved in 1-2, 1-3, 1-4 interactions within the molecular topology, their pairwise interaction may be turned off, and thus they may not appear in the neighbor list, and will not be part of the local data created by this command. More specifically, this will be true of I,J pairs with a weighting factor of 0.0; pairs with a non-zero weighting factor are included. The weighting factors for 1-2, 1-3, and 1-4 pairwise interactions are set by the *special_bonds* command. An exception is if long-range Coulombics are being computed via the *kspace_style* command, then atom pairs with weighting factors of zero are still included in the neighbor list, so that a portion of the long-range interaction contribution can be computed in the pair style. Hence in that case, those atom pairs will be part of the local data created by this command.

Output info:

This compute calculates a local vector or local array depending on the number of keywords. The length of the vector or number of rows in the array is the number of pairs. If a single keyword is specified, a local vector is produced. If two or more keywords are specified, a local array is produced where the number of columns = the number of keywords. The vector or array can be accessed by any command that uses local values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The output for *dist* will be in distance *units*. The output for *eng* will be in energy *units*. The output for *force*, *fx*, *fy*, and *fz* will be in force *units*. The output for *pN* will be in whatever units the pair style defines.

17.65.4 Restrictions

none

17.65.5 Related commands

dump local, *compute property/local*

17.65.6 Default

The keyword default is cutoff = type.

17.66 compute pe command

17.66.1 Syntax

```
compute ID group-ID pe keyword ...
```

- ID, group-ID are documented in *compute* command
- pe = style name of this compute command
- zero or more keywords may be appended
- keyword = *pair* or *bond* or *angle* or *dihedral* or *improper* or *kspace* or *fix*

17.66.2 Examples

```
compute 1 all pe
compute molPE all pe bond angle dihedral improper
```

17.66.3 Description

Define a computation that calculates the potential energy of the entire system of atoms. The specified group must be "all". See the *compute pe/atom* command if you want per-atom energies. These per-atom values could be summed for a group of atoms via the *compute reduce* command.

The energy is calculated by the various pair, bond, etc potentials defined for the simulation. If no extra keywords are listed, then the potential energy is the sum of pair, bond, angle, dihedral, improper, kspace (long-range), and fix energy. I.e. it is as if all the keywords were listed. If any extra keywords are listed, then only those components are summed to compute the potential energy.

The Kspace contribution requires 1 extra FFT each timestep the energy is calculated, if using the PPPM solver via the *kspace_style pppm* command. Thus it can increase the cost of the PPPM calculation if it is needed on a large fraction of the simulation timesteps.

Various fixes can contribute to the total potential energy of the system if the *fix* contribution is included. See the doc pages for *individual fixes* for details of which ones compute a potential energy.

Note: The *fix_modify energy yes* command must also be specified if a fix is to contribute potential energy to this command.

A compute of this style with the ID of "thermo_pe" is created when LAMMPS starts up, as if this command were in the input script:

```
compute thermo_pe all pe
```

See the "thermo_style" command for more details.

Output info:

This compute calculates a global scalar (the potential energy). This value can be used by any command that uses a global scalar value from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy *units*.

17.66.4 Restrictions

none

17.66.5 Related commands

compute pe/atom

Default: none

17.67 compute pe/atom command

17.67.1 Syntax

```
compute ID group-ID pe/atom keyword ...
```

- ID, group-ID are documented in *compute* command
- pe/atom = style name of this compute command
- zero or more keywords may be appended
- keyword = *pair* or *bond* or *angle* or *dihedral* or *improper* or *kspace* or *fix*

17.67.2 Examples

```
compute 1 all pe/atom
compute 1 all pe/atom pair
compute 1 all pe/atom pair bond
```

17.67.3 Description

Define a computation that computes the per-atom potential energy for each atom in a group. See the *compute pe* command if you want the potential energy of the entire system.

The per-atom energy is calculated by the various pair, bond, etc potentials defined for the simulation. If no extra keywords are listed, then the potential energy is the sum of pair, bond, angle, dihedral,improper, kspace (long-range), and fix energy. I.e. it is as if all the keywords were listed. If any extra keywords are listed, then only those components are summed to compute the potential energy.

Note that the energy of each atom is due to its interaction with all other atoms in the simulation, not just with other atoms in the group.

For an energy contribution produced by a small set of atoms (e.g. 4 atoms in a dihedral or 3 atoms in a Tersoff 3-body interaction), that energy is assigned in equal portions to each atom in the set. E.g. 1/4 of the dihedral energy to each of the 4 atoms.

The *dihedral_style charmm* style calculates pairwise interactions between 1-4 atoms. The energy contribution of these terms is included in the pair energy, not the dihedral energy.

The KSpace contribution is calculated using the method in *(Heyes)* for the Ewald method and a related method for PPPM, as specified by the *kspace_style pppm* command. For PPPM, the calculation requires 1 extra FFT each timestep that per-atom energy is calculated. This document describes how the long-range per-atom energy calculation is performed.

Various fixes can contribute to the per-atom potential energy of the system if the *fix* contribution is included. See the doc pages for *individual fixes* for details of which ones compute a per-atom potential energy.

Note: The *fix_modify energy yes* command must also be specified if a fix is to contribute per-atom potential energy to this command.

As an example of per-atom potential energy compared to total potential energy, these lines in an input script should yield the same result in the last 2 columns of thermo output:

```
compute        peratom all pe/atom
compute        pe all reduce sum c_peratom
thermo_style   custom step temp etotal press pe c_pe
```

Note: The per-atom energy does not include any Lennard-Jones tail corrections to the energy added by the *pair_modify tail yes* command, since those are contributions to the global system energy.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values will be in energy *units*.

17.67.4 Restrictions

17.67.5 Related commands

compute pe, *compute stress/atom*

Default: none

(Heyes) Heyes, Phys Rev B 49, 755 (1994),

17.68 compute plasticity/atom command

17.68.1 Syntax

```
compute ID group-ID plasticity/atom
```

- ID, group-ID are documented in compute command
- plasticity/atom = style name of this compute command

17.68.2 Examples

```
compute 1 all plasticity/atom
```

17.68.3 Description

Define a computation that calculates the per-atom plasticity for each atom in a group. This is a quantity relevant for *Peridynamics models*. See this document for an overview of LAMMPS commands for Peridynamics modeling.

The plasticity for a Peridynamic particle is the so-called consistency parameter (lambda). For elastic deformation lambda = 0, otherwise lambda > 0 for plastic deformation. For details, see *(Mitchell)* and the PDF doc included in the LAMMPS distribution in doc/PDF/PDLammps_EPS.pdf.

This command can be invoked for one of the Peridynamic *pair styles*: peri/eps.

The plasticity value will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values are unitless numbers (lambda) >= 0.0.

17.68.4 Restrictions

This compute is part of the PERI package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.68.5 Related commands

compute damage/atom, *compute dilatation/atom*

Default: none

(Mitchell) Mitchell, "A non-local, ordinary-state-based viscoelasticity model for peridynamics", Sandia National Lab Report, 8064:1-28 (2011).

17.69 compute pressure command

17.69.1 Syntax

```
compute ID group-ID pressure temp-ID keyword ...
```

- ID, group-ID are documented in *compute* command
- pressure = style name of this compute command
- temp-ID = ID of compute that calculates temperature, can be NULL if not needed
- zero or more keywords may be appended
- keyword = *ke* or *pair* or *bond* or *angle* or *dihedral* or *improper* or *kspace* or *fix* or *virial* or *pair/hybrid*

17.69.2 Examples

```
compute 1 all pressure thermo_temp
compute 1 all pressure NULL pair bond
compute 1 all pressure NULL pair/hybrid lj/cut
```

17.69.3 Description

Define a computation that calculates the pressure of the entire system of atoms. The specified group must be "all". See the *compute stress/atom* command if you want per-atom pressure (stress). These per-atom values could be summed for a group of atoms via the *compute reduce* command.

The pressure is computed by the formula

$$P = \frac{Nk_BT}{V} + \frac{\sum_i^{N'} r_i \bullet f_i}{dV}$$

where *N* is the number of atoms in the system (see discussion of DOF below), k_B is the Boltzmann constant, *T* is the temperature, d is the dimensionality of the system (2 or 3 for 2d/3d), and *V* is the system volume (or area in 2d). The second term is the virial, equal to -dU/dV, computed for all pairwise as well as 2-body, 3-body, 4-body, many-body, and long-range interactions, where r_i and f_i are the position and force vector of atom *i*, and the black dot indicates a dot product. When periodic boundary conditions are used, N' necessarily includes periodic image (ghost) atoms outside the central box, and the position and force vectors of ghost atoms are thus included in the summation. When periodic boundary conditions are not used, N' = N = the number of atoms in the system. *Fixes* that impose constraints (e.g. the *fix shake* command) also contribute to the virial term.

A symmetric pressure tensor, stored as a 6-element vector, is also calculated by this compute. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz. The equation for the I,J components (where I and J = x,y,z) is similar to the above formula, except that the first term uses components of the kinetic energy tensor and the second term uses components of the virial tensor:

$$P_{IJ} = \frac{\sum_k^N m_k v_{k_I} v_{k_J}}{V} + \frac{\sum_k^{N'} r_{k_I} f_{k_J}}{V}$$

If no extra keywords are listed, the entire equations above are calculated. This includes a kinetic energy (temperature) term and the virial as the sum of pair, bond, angle, dihedral, improper, kspace (long-range), and fix contributions to the force on each atom. If any extra keywords are listed, then only those components are summed to compute temperature or ke and/or the virial. The *virial* keyword means include all terms except the kinetic energy *ke*.

The *pair/hybrid* keyword means to only include contribution from a sub-style in a *hybrid* or *hybrid/overlay* pair style.

Details of how LAMMPS computes the virial efficiently for the entire system, including for many-body potentials and accounting for the effects of periodic boundary conditions are discussed in *(Thompson)*.

The temperature and kinetic energy tensor is not calculated by this compute, but rather by the temperature compute specified with the command. If the kinetic energy is not included in the pressure, than the temperature compute is not used and can be specified as NULL. Normally the temperature compute used by compute pressure should calculate the temperature of all atoms for consistency with the virial term, but any compute style that calculates temperature can be used, e.g. one that excludes frozen atoms or other degrees of freedom.

Note that if desired the specified temperature compute can be one that subtracts off a bias to calculate a temperature using only the thermal velocity of the atoms, e.g. by subtracting a background streaming velocity. See the doc pages for individual *compute commands* to determine which ones include a bias.

Also note that the N in the first formula above is really degrees-of-freedom divided by d = dimensionality, where the DOF value is calculated by the temperature compute. See the various *compute temperature* styles for details.

A compute of this style with the ID of "thermo_press" is created when LAMMPS starts up, as if this command were in the input script:

```
compute thermo_press all pressure thermo_temp
```

where "thermo_temp" is the ID of a similarly defined compute of style "temp". See the "thermo_style" command for more details.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Output info:

This compute calculates a global scalar (the pressure) and a global vector of length 6 (pressure tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar and vector values calculated by this compute are "intensive". The scalar and vector values will be in pressure *units*.

17.69.4 Restrictions

none

17.69.5 Related commands

compute temp, *compute stress/atom*, *thermo_style*,

Default: none

(Thompson) Thompson, Plimpton, Mattson, J Chem Phys, 131, 154107 (2009).

17.70 compute pressure/cylinder command

17.70.1 Syntax

```
compute ID group-ID pressure/cylinder zlo zhi Rmax bin_width
```

- ID, group-ID are documented in *compute* command
- pressure/cylinder = style name of this compute command

- zlo = minimum z-boundary for cylinder
- zhi = maximum z-boundary for cylinder
- Rmax = maximum radius to perform calculation to
- bin_width = width of radial bins to use for calculation

17.70.2 Examples

```
compute 1 all pressure/cylinder -10.0 10.0 15.0 0.25
```

17.70.3 Description

Define a computation that calculates the pressure tensor of a system in cylindrical coordinates, as discussed in *(Addington)*. This is useful for systems with a single axis of rotational symmetry, such as cylindrical micelles or carbon nanotubes. The compute splits the system into radial, cylindrical-shell-type bins of width bin_width, centered at x=0,y=0, and calculates the radial (P_rhorho), azimuthal (P_phiphi), and axial (P_zz) components of the configurational pressure tensor. The local density is also calculated for each bin, so that the true pressure can be recovered as P_kin+P_conf=density*k*T+P_conf. The output is a global array with 5 columns; one each for bin radius, local number density, P_rhorho, P_phiphi, and P_zz. The number of rows is governed by the values of Rmax and bin_width. Pressure tensor values are output in pressure units.

Output info:

This compute calculates a global array with 5 columns and Rmax/bin_width rows. The output columns are: R (distance units), number density (inverse volume units), configurational radial pressure (pressure units), configurational azimuthal pressure (pressure units), and configurational axial pressure (pressure units).

The values calculated by this compute are "intensive". The pressure values will be in pressure *units*. The number density values will be in inverse volume *units*.

17.70.4 Restrictions

This compute currently calculates the pressure tensor contributions for pair styles only (i.e. no bond, angle, dihedral, etc. contributions and in the presence of bonded interactions, the result will be incorrect due to exclusions for special bonds) and requires pair-wise force calculations not available for most many-body pair styles. K-space calculations are also excluded. Note that this pressure compute outputs the configurational terms only; the kinetic contribution is not included and may be calculated from the number density output by P_kin=density*k*T.

This compute is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.70.5 Related commands

compute temp, *compute stress/atom*, *thermo_style*,

Default: none

(Addington) Addington, Long, Gubbins, J Chem Phys, 149, 084109 (2018).

17.71 compute pressure/uef command

17.71.1 Syntax

```
compute ID group-ID pressure/uef temp-ID keyword ...
```

- ID, group-ID are documented in *compute* command
- pressure/uef = style name of this compute command
- temp-ID = ID of compute that calculates temperature, can be NULL if not needed
- zero or more keywords may be appended
- keyword = *ke* or *pair* or *bond* or *angle* or *dihedral* or *improper* or *kspace* or *fix* or *virial*

17.71.2 Examples

```
compute 1 all pressure/uef my_temp_uef
compute 2 all pressure/uef my_temp_uef virial
```

17.71.3 Description

This command is used to compute the pressure tensor in the reference frame of the applied flow field when *fix nvt/uef* or *fix npt/uef* is used. It is not necessary to use this command to compute the scalar value of the pressure. A *compute pressure* may be used for that purpose.

The keywords and output information are documented in *compute_pressure*.

17.71.4 Restrictions

This fix is part of the USER-UEF package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This command can only be used when *fix nvt/uef* or *fix npt/uef* is active.

The kinetic contribution to the pressure tensor will be accurate only when the compute specified by *temp-ID* is a *compute temp/uef*.

17.71.5 Related commands

compute pressure, *fix nvt/uef*, *compute temp/uef*

Default: none

17.72 compute property/atom command

17.72.1 Syntax

```
compute ID group-ID property/atom input1 input2 ...
```

- ID, group-ID are documented in *compute* command
- property/atom = style name of this compute command
- input = one or more atom attributes

```
possible attributes = id, mol, proc, type, mass,
                      x, y, z, xs, ys, zs, xu, yu, zu, ix, iy, iz,
                      vx, vy, vz, fx, fy, fz,
                      q, mux, muy, muz, mu,
                      sp, spx, spy, spz, fmx, fmy, fmz,
                      radius, diameter, omegax, omegay, omegaz,
                      angmomx, angmomy, angmomz,
                      shapex,shapey, shapez,
                      quatw, quati, quatj, quatk, tqx, tqy, tqz,
                      end1x, end1y, end1z, end2x, end2y, end2z,
                      corner1x, corner1y, corner1z,
                      corner2x, corner2y, corner2z,
                      corner3x, corner3y, corner3z,
                      nbonds,
                      vfrac, s0,
                      spin, eradius, ervel, erforce,
                      rho, drho, e, de, cv,
                      i_name, d_name
```

```
id = atom ID
mol = molecule ID
proc = ID of processor that owns atom
type = atom type
mass = atom mass
x,y,z = unscaled atom coordinates
xs,ys,zs = scaled atom coordinates
xu,yu,zu = unwrapped atom coordinates
ix,iy,iz = box image that the atom is in
vx,vy,vz = atom velocities
fx,fy,fz = forces on atoms
q = atom charge
mux,muy,muz = orientation of dipole moment of atom
mu = magnitude of dipole moment of atom
sp = atomic magnetic spin moment
spx, spy, spz = direction of the atomic magnetic spin
fmx, fmy, fmz = magnetic force
radius,diameter = radius,diameter of spherical particle
omegax,omegay,omegaz = angular velocity of spherical particle
angmomx,angmomy,angmomz = angular momentum of aspherical particle
shapex,shapey,shapez = 3 diameters of aspherical particle
quatw,quati,quatj,quatk = quaternion components for aspherical or body particles
tqx,tqy,tqz = torque on finite-size particles
end12x, end12y, end12z = end points of line segment
corner123x, corner123y, corner123z = corner points of triangle
nbonds = number of bonds assigned to an atom
```

```
PERI package per-atom properties:
vfrac = ???
s0 = ???
```

```
USER-EFF and USER-AWPMD package per-atom properties:
spin = electron spin
eradius = electron radius
ervel = electron radial velocity
erforce = electron radial force
```

```
USER-SPH package per-atom properties:
rho = ???
drho = ???
e = ???
de = ???
cv = ???
```

```
fix property/atom per-atom properties:
i_name = custom integer vector with name
d_name = custom integer vector with name
```

17.72.2 Examples

```
compute 1 all property/atom xs vx fx mux
compute 2 all property/atom type
compute 1 all property/atom ix iy iz
compute 3 all property/atom sp spx spy spz
```

17.72.3 Description

Define a computation that simply stores atom attributes for each atom in the group. This is useful so that the values can be used by other *output commands* that take computes as inputs. See for example, the *compute reduce*, *fix ave/atom*, *fix ave/histo*, *fix ave/chunk*, and *atom-style variable* commands.

The list of possible attributes is the same as that used by the *dump custom* command, which describes their meaning, with some additional quantities that are only defined for certain *atom styles*. Basically, this augmented list gives an input script access to any per-atom quantity stored by LAMMPS.

The values are stored in a per-atom vector or array as discussed below. Zeroes are stored for atoms not in the specified group or for quantities that are not defined for a particular particle in the group (e.g. *shapex* if the particle is not an ellipsoid).

The additional quantities only accessible via this command, and not directly via the *dump custom* command, are as follows.

Shapex, *shapey*, and *shapez* are defined for ellipsoidal particles and define the 3d shape of each particle.

Quatw, *quati*, *quatj*, and *quatk* are defined for ellipsoidal particles and body particles and store the 4-vector quaternion representing the orientation of each particle. See the *set* command for an explanation of the quaternion vector.

End1x, *end1y*, *end1z*, *end2x*, *end2y*, *end2z*, are defined for line segment particles and define the end points of each line segment.

Corner1x, *corner1y*, *corner1z*, *corner2x*, *corner2y*, *corner2z*, *corner3x*, *corner3y*, *corner3z*, are defined for triangular particles and define the corner points of each triangle.

Nbonds is available for all molecular atom styles and refers to the number of explicit bonds assigned to an atom. Note that if the *newton bond* command is set to *on*, which is the default, then every bond in the system is assigned to only one of the two atoms in the bond. Thus a bond between atoms I,J may be tallied for either atom I or atom J. If *newton bond off* is set, it will be tallied with both atom I and atom J.

The *i_name* and *d_name* attributes refer to custom integer and floating-point properties that have been added to each atom via the *fix property/atom* command. When that command is used specific names are given to each attribute which are what is specified as the "name" portion of *i_name* or *d_name*.

Output info:

This compute calculates a per-atom vector or per-atom array depending on the number of input values. If a single input is specified, a per-atom vector is produced. If two or more inputs are specified, a per-atom array is produced where the number of columns = the number of inputs. The vector or array can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector or array values will be in whatever *units* the corresponding attribute is in, e.g. velocity units for vx, charge units for q, etc.

For the spin quantities, sp is in the units of the Bohr magneton, spx, spy, and spz are unitless quantities, and fmx, fmy and fmz are given in rad/THz.

17.72.4 Restrictions

none

17.72.5 Related commands

dump custom, *compute reduce*, *fix ave/atom*, *fix ave/chunk*, *fix property/atom*

Default: none

17.73 compute property/chunk command

17.73.1 Syntax

```
compute ID group-ID property/chunk chunkID input1 input2 ...
```

- ID, group-ID are documented in *compute* command
- property/chunk = style name of this compute command
- input = one or more attributes

```
attributes = count, id, coord1, coord2, coord3
  count = # of atoms in chunk
  id = original chunk IDs before compression by compute chunk/atom
  coord123 = coordinates for spatial bins calculated by compute chunk/atom
```

17.73.2 Examples

```
compute 1 all property/chunk count
compute 1 all property/chunk ID coord1
```

17.73.3 Description

Define a computation that stores the specified attributes of chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a *compute chunk/atom* command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the *compute chunk/atom* and *Howto chunk* doc pages for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

This compute calculates and stores the specified attributes of chunks as global data so they can be accessed by other *output commands* and used in conjunction with other commands that generate per-chunk data, such as *compute com/chunk* or *compute msd/chunk*.

Note that only atoms in the specified group contribute to the calculation of the *count* attribute. The *compute chunk/atom* command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

The *count* attribute is the number of atoms in the chunk.

The *id* attribute stores the original chunk ID for each chunk. It can only be used if the *compress* keyword was set to *yes* for the *compute chunk/atom* command referenced by chunkID. This means that the original chunk IDs (e.g. molecule IDs) will have been compressed to remove chunk IDs with no atoms assigned to them. Thus a compressed chunk ID of 3 may correspond to an original chunk ID (molecule ID in this case) of 415. The *id* attribute will then be 415 for the 3rd chunk.

The *coordN* attributes can only be used if a *binning* style was used in the *compute chunk/atom* command referenced by chunkID. For *bin/1d*, *bin/2d*, and *bin/3d* styles the attribute is the center point of the bin in the corresponding dimension. Style *bin/1d* only defines a *coord1* attribute. Style *bin/2d* adds a *coord2* attribute. Style *bin/3d* adds a *coord3* attribute.

Note that if the value of the *units* keyword used in the *compute chunk/atom command* is *box* or *lattice*, the *coordN* attributes will be in distance *units*. If the value of the *units* keyword is *reduced*, the *coordN* attributes will be in unitless reduced units (0-1).

The simplest way to output the results of the compute property/chunk calculation to a file is to use the *fix ave/time* command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk1 all property/chunk cc1 count
compute myChunk2 all com/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk1 c_myChunk2[*] file tmp.out mode vector
```

Output info:

This compute calculates a global vector or global array depending on the number of input values. The length of the vector or number of rows in the array is the number of chunks.

This compute calculates a global vector or global array where the number of rows = the number of chunks *Nchunk* as calculated by the specified *compute chunk/atom* command. If a single input is specified, a global vector is produced. If two or more inputs are specified, a global array is produced where the number of columns = the number of inputs. The vector or array can be accessed by any command that uses global values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector or array values are "intensive". The values will be unitless or in the units discussed above.

17.73.4 Restrictions

none

17.73.5 Related commands

fix ave/chunk

Default: none

17.74 compute property/local command

17.74.1 Syntax

```
compute ID group-ID property/local attribute1 attribute2 ... keyword args ...
```

- ID, group-ID are documented in *compute* command
- property/local = style name of this compute command
- one or more attributes may be appended

```
possible attributes = natom1 natom2 ntype1 ntype2
                      patom1 patom2 ptype1 ptype2
                      batom1 batom2 btype
                      aatom1 aatom2 aatom3 atype
                      datom1 datom2 datom3 datom4 dtype
                      iatom1 iatom2 iatom3 iatom4 itype
```

```
natom1, natom2 = IDs of 2 atoms in each pair (within neighbor cutoff)
ntype1, ntype2 = type of 2 atoms in each pair (within neighbor cutoff)
patom1, patom2 = IDs of 2 atoms in each pair (within force cutoff)
ptype1, ptype2 = type of 2 atoms in each pair (within force cutoff)
batom1, batom2 = IDs of 2 atoms in each bond
btype = bond type of each bond
aatom1, aatom2, aatom3 = IDs of 3 atoms in each angle
atype = angle type of each angle
datom1, datom2, datom3, datom4 = IDs of 4 atoms in each dihedral
dtype = dihedral type of each dihedral
iatom1, iatom2, iatom3, iatom4 = IDs of 4 atoms in each improper
itype = improper type of each improper
```

- zero or more keyword/arg pairs may be appended
- keyword = *cutoff*

  cutoff arg = *type* or *radius*

17.74.2 Examples

```
compute 1 all property/local btype batom1 batom2
compute 1 all property/local atype aatom2
```

17.74.3 Description

Define a computation that stores the specified attributes as local data so it can be accessed by other *output commands*. If the input attributes refer to bond information, then the number of datums generated, aggregated across all processors, equals the number of bonds in the system. Ditto for pairs, angles, etc.

If multiple attributes are specified then they must all generate the same amount of information, so that the resulting local array has the same number of rows for each column. This means that only bond attributes can be specified together, or angle attributes, etc. Bond and angle attributes can not be mixed in the same compute property/local command.

If the inputs are pair attributes, the local data is generated by looping over the pairwise neighbor list. Info about an individual pairwise interaction will only be included if both atoms in the pair are in the specified compute group. For *natom1* and *natom2*, all atom pairs in the neighbor list are considered (out to the neighbor cutoff = force cutoff + *neighbor skin*). For *patom1* and *patom2*, the distance between the atoms must be less than the force cutoff distance for that pair to be included, as defined by the *pair_style* and *pair_coeff* commands.

The optional *cutoff* keyword determines how the force cutoff distance for an interaction is determined for the *patom1* and *patom2* attributes. For the default setting of *type*, the pairwise cutoff defined by the *pair_style* command for the types of the two atoms is used. For the *radius* setting, the sum of the radii of the two particles is used as a cutoff. For example, this is appropriate for granular particles which only interact when they are overlapping, as computed by *granular pair styles*. Note that if a granular model defines atom types such that all particles of a specific type are monodisperse (same diameter), then the two settings are effectively identical.

If the inputs are bond, angle, etc attributes, the local data is generated by looping over all the atoms owned on a processor and extracting bond, angle, etc info. For bonds, info about an individual bond will only be included if both atoms in the bond are in the specified compute group. Likewise for angles, dihedrals, etc.

For bonds and angles, a bonds/angles that have been broken by setting their bond/angle type to 0 will not be included. Bonds/angles that have been turned off (see the *fix shake* or *delete_bonds* commands) by setting their bond/angle type negative are written into the file. This is consistent with the *compute bond/local* and *compute angle/local* commands

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For example, output from the *compute bond/local* command can be combined with bond atom indices from this command and output by the *dump local* command in a consistent way.

The *natom1* and *natom2*, or *patom1* and *patom2* attributes refer to the atom IDs of the 2 atoms in each pairwise interaction computed by the *pair_style* command. The *ntype1* and *ntype2*, or *ptype1* and *ptype2* attributes refer to the atom types of the 2 atoms in each pairwise interaction.

Note: For pairs, if two atoms I,J are involved in 1-2, 1-3, 1-4 interactions within the molecular topology, their pairwise interaction may be turned off, and thus they may not appear in the neighbor list, and will not be part of the local data created by this command. More specifically, this may be true of I,J pairs with a weighting factor of 0.0; pairs with a non-zero weighting factor are included. The weighting factors for 1-2, 1-3, and 1-4 pairwise interactions are set by the *special_bonds* command.

The *batom1* and *batom2* attributes refer to the atom IDs of the 2 atoms in each *bond*. The *btype* attribute refers to the type of the bond, from 1 to Nbtypes = # of bond types. The number of bond types is defined in the data file read by

the *read_data* command.

The attributes that start with "a", "d", "i", refer to similar values for *angles*, *dihedrals*, and *impropers*.

Output info:

This compute calculates a local vector or local array depending on the number of input values. The length of the vector or number of rows in the array is the number of bonds, angles, etc. If a single input is specified, a local vector is produced. If two or more inputs are specified, a local array is produced where the number of columns = the number of inputs. The vector or array can be accessed by any command that uses local values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector or array values will be integers that correspond to the specified attribute.

17.74.4 Restrictions

none

17.74.5 Related commands

dump local, *compute reduce*

17.74.6 Default

The keyword default is cutoff = type.

17.75 compute ptm/atom command

17.75.1 Syntax

```
compute ID group-ID ptm/atom structures threshold group2-ID
```

- ID, group-ID are documented in *compute* command
- ptm/atom = style name of this compute command
- structures = structure types to search for
- threshold = lattice distortion threshold (RMSD)
- group2-ID determines which group is used for neighbor selection (optional, default "all")

17.75.2 Examples

```
compute 1 all ptm/atom default 0.1 all
compute 1 all ptm/atom fcc-hcp-dcub-dhex 0.15 all
compute 1 all ptm/atom all 0
```

17.75.3 Description

Define a computation that determines the local lattice structure around an atom using the PTM (Polyhedral Template Matching) method. The PTM method is described in *(Larsen)*.

Currently, there are seven lattice structures PTM recognizes:

- fcc = 1
- hcp = 2
- bcc = 3
- ico (icosahedral) = 4
- sc (simple cubic) = 5
- dcub (diamond cubic) = 6
- dhex (diamond hexagonal) = 7
- graphene = 8

The value of the PTM structure will be 0 for unknown types and -1 for atoms not in the specified compute group. The choice of structures to search for can be specified using the "structures" argument, which is a hyphen-separated list of structure keywords. Two convenient pre-set options are provided:

- default: fcc-hcp-bcc-ico
- all: fcc-hcp-bcc-ico-sc-dcub-dhex-graphene

The 'default' setting detects the same structures as the Common Neighbor Analysis method. The 'all' setting searches for all structure types. A performance penalty is incurred for the diamond and graphene structures, so it is not recommended to use this option if it is known that the simulation does not contain these structures.

PTM identifies structures using two steps. First, a graph isomorphism test is used to identify potential structure matches. Next, the deviation is computed between the local structure (in the simulation) and a template of the ideal lattice structure. The deviation is calculated as:

$$\mathrm{RMSD}(\mathbf{u},\mathbf{v}) = \min_{s,\mathbf{Q}} \sqrt{\frac{1}{N}\sum_{i=1}^{N} ||s[\vec{u_i} - \overline{\mathbf{u}}] - \mathbf{Q}\vec{v_i}||^2}$$

Here, u and v contain the coordinates of the local and ideal structures respectively, s is a scale factor, and Q is a rotation. The best match is identified by the lowest RMSD value, using the optimal scaling, rotation, and correspondence between the points.

The 'threshold' keyword sets an upper limit on the maximum permitted deviation before a local structure is identified as disordered. Typical values are in the range 0.1-0.15, but larger values may be desirable at higher temperatures. A value of 0 is equivalent to infinity and can be used if no threshold is desired.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (e.g. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently or to have multiple compute/dump commands, each with a *ptm/atom* style. By default the compute processes **all** neighbors unless the optional *group2-ID* argument is given, then only members of that group are considered as neighbors.

Output info:

This compute calculates a per-atom array, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

Results are stored in the per-atom array in the following order:

- type

- rmsd
- interatomic distance
- qw
- qx
- qy
- qz

The type is a number from -1 to 8. The rmsd is a positive real number. The interatomic distance is computed from the scale factor in the RMSD equation. The (qw,qx,qy,qz) parameters represent the orientation of the local structure in quaternion form. The reference coordinates for each template (from which the orientation is determined) can be found in the *ptm_constants.h* file in the PTM source directory. For atoms that are not within the compute group-ID, all values are set to zero.

17.75.4 Restrictions

This fix is part of the USER-PTM package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.75.5 Related commands

compute centro/atom compute cna/atom

Default: none

(Larsen) Larsen, Schmidt, Schiotz, Modelling Simul Mater Sci Eng, 24, 055007 (2016).

17.76 compute rdf command

17.76.1 Syntax

```
compute ID group-ID rdf Nbin itype1 jtype1 itype2 jtype2 ... keyword/value ...
```

- ID, group-ID are documented in *compute* command
- rdf = style name of this compute command
- Nbin = number of RDF bins
- itypeN = central atom type for Nth RDF histogram (see asterisk form below)
- jtypeN = distribution atom type for Nth RDF histogram (see asterisk form below)
- zero or more keyword/value pairs may be appended
- keyword = *cutoff*

  ```
  cutoff value = Rcut
    Rcut = cutoff distance for RDF computation (distance units)
  ```

17.76.2 Examples

```
compute 1 all rdf 100
compute 1 all rdf 100 1 1
compute 1 all rdf 100 * 3 cutoff 5.0
compute 1 fluid rdf 500 1 1 1 2 2 1 2 2
compute 1 fluid rdf 500 1*3 2 5 *10 cutoff 3.5
```

17.76.3 Description

Define a computation that calculates the radial distribution function (RDF), also called g(r), and the coordination number for a group of particles. Both are calculated in histogram form by binning pairwise distances into *Nbin* bins from 0.0 to the maximum force cutoff defined by the *pair_style* command or the cutoff distance *Rcut* specified via the *cutoff* keyword. The bins are of uniform size in radial distance. Thus a single bin encompasses a thin shell of distances in 3d and a thin ring of distances in 2d.

Note: If you have a bonded system, then the settings of *special_bonds* command can remove pairwise interactions between atoms in the same bond, angle, or dihedral. This is the default setting for the *special_bonds* command, and means those pairwise interactions do not appear in the neighbor list. Because this fix uses a neighbor list, it also means those pairs will not be included in the RDF. This does not apply when using long-range coulomb interactions (*coul/long*, *coul/msm*, *coul/wolf* or similar. One way to get around this would be to set special_bond scaling factors to very tiny numbers that are not exactly zero (e.g. 1.0e-50). Another workaround is to write a dump file, and use the *rerun* command to compute the RDF for snapshots in the dump file. The rerun script can use a *special_bonds* command that includes all pairs in the neighbor list.

By default the RDF is computed out to the maximum force cutoff defined by the *pair_style* command. If the *cutoff* keyword is used, then the RDF is computed accurately out to the *Rcut* > 0.0 distance specified.

Note: Normally, you should only use the *cutoff* keyword if no pair style is defined, e.g. the *rerun* command is being used to post-process a dump file of snapshots. Or if you really want the RDF for distances beyond the pair_style force cutoff and cannot easily post-process a dump file to calculate it. This is because using the *cutoff* keyword incurs extra computation and possibly communication, which may slow down your simulation. If you specify a *Rcut* <= force cutoff, you will force an additional neighbor list to be built at every timestep this command is invoked (or every reneighboring timestep, whichever is less frequent), which is inefficient. LAMMPS will warn you if this is the case. If you specify a *Rcut* > force cutoff, you must insure ghost atom information out to *Rcut* + *skin* is communicated, via the *comm_modify cutoff* command, else the RDF computation cannot be performed, and LAMMPS will give an error message. The *skin* value is what is specified with the *neighbor* command. In this case, you are forcing a large neighbor list to be built just for the RDF computation, and extra communication to be performed every timestep.

The *itypeN* and *jtypeN* arguments are optional. These arguments must come in pairs. If no pairs are listed, then a single histogram is computed for g(r) between all atom types. If one or more pairs are listed, then a separate histogram is generated for each *itype*,*jtype* pair.

The *itypeN* and *jtypeN* settings can be specified in one of two ways. An explicit numeric value can be used, as in the 4th example above. Or a wild-card asterisk can be used to specify a range of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

If both *itypeN* and *jtypeN* are single values, as in the 4th example above, this means that a g(r) is computed where atoms of type *itypeN* are the central atom, and atoms of type *jtypeN* are the distribution atom. If either *itypeN* and *jtypeN* represent a range of values via the wild-card asterisk, as in the 5th example above, this means that a g(r) is

computed where atoms of any of the range of types represented by *itypeN* are the central atom, and atoms of any of the range of types represented by *jtypeN* are the distribution atom.

Pairwise distances are generated by looping over a pairwise neighbor list, just as they would be in a *pair_style* computation. The distance between two atoms I and J is included in a specific histogram if the following criteria are met:

- atoms I,J are both in the specified compute group
- the distance between atoms I,J is less than the maximum force cutoff
- the type of the I atom matches itypeN (one or a range of types)
- the type of the J atom matches jtypeN (one or a range of types)

It is OK if a particular pairwise distance is included in more than one individual histogram, due to the way the *itypeN* and *jtypeN* arguments are specified.

The g(r) value for a bin is calculated from the histogram count by scaling it by the idealized number of how many counts there would be if atoms of type *jtypeN* were uniformly distributed. Thus it involves the count of *itypeN* atoms, the count of *jtypeN* atoms, the volume of the entire simulation box, and the volume of the bin's thin shell in 3d (or the area of the bin's thin ring in 2d).

A coordination number coord(r) is also calculated, which is the number of atoms of type *jtypeN* within the current bin or closer, averaged over atoms of type *itypeN*. This is calculated as the area- or volume-weighted sum of g(r) values over all bins up to and including the current bin, multiplied by the global average volume density of atoms of type jtypeN.

The simplest way to output the results of the compute rdf calculation to a file is to use the *fix ave/time* command, for example:

```
compute myRDF all rdf 50
fix 1 all ave/time 100 1 100 c_myRDF[*] file tmp.rdf mode vector
```

Output info:

This compute calculates a global array with the number of rows = *Nbins*, and the number of columns = 1 + 2*Npairs, where Npairs is the number of I,J pairings specified. The first column has the bin coordinate (center of the bin), Each successive set of 2 columns has the g(r) and coord(r) values for a specific set of *itypeN* versus *jtypeN* interactions, as described above. These values can be used by any command that uses a global values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The array values calculated by this compute are all "intensive".

The first column of array values will be in distance *units*. The g(r) columns of array values are normalized numbers >= 0.0. The coordination number columns of array values are also numbers >= 0.0.

17.76.4 Restrictions

The RDF is not computed for distances longer than the force cutoff, since processors (in parallel) don't know about atom coordinates for atoms further away than that distance. If you want an RDF for larger distances, you can use the *rerun* command to post-process a dump file and set the cutoff for the potential to be longer in the rerun script. Note that in the rerun context, the force cutoff is arbitrary, since you aren't running dynamics and thus are not changing your model. The definition of g(r) used by LAMMPS is only appropriate for characterizing atoms that are uniformly distributed throughout the simulation cell. In such cases, the coordination number is still correct and meaningful. As an example, if a large simulation cell contains only one atom of type *itypeN* and one of *jtypeN*, then g(r) will register an arbitrarily large spike at whatever distance they happen to be at, and zero everywhere else. Coord(r) will show a step change from zero to one at the location of the spike in g(r).

Note: compute rdf can handle dynamic groups and systems where atoms are added or removed, but this causes that certain normalization parameters need to be re-computed in every step and include collective communication operations. This will reduce performance and limit parallel efficiency and scaling. For systems, where only the type of atoms changes (e.g. when using *fix atom/swap*), you need to explicitly request the dynamic normalization updates via *compute_modify dynamic yes*

17.76.5 Related commands

fix ave/time, *compute_modify*, *compute adf*

17.76.6 Default

The keyword defaults are cutoff = 0.0 (use the pairwise force cutoff).

17.77 compute reduce command

17.78 compute reduce/region command

17.78.1 Syntax

```
compute ID group-ID style arg mode input1 input2 ... keyword args ...
```

- ID, group-ID are documented in *compute* command
- style = *reduce* or *reduce/region*

  ```
  reduce arg = none
  reduce/region arg = region-ID
    region-ID = ID of region to use for choosing atoms
  ```

- mode = *sum* or *min* or *max* or *ave* or *sumsq* or *avesq*
- one or more inputs can be listed
- input = x, y, z, vx, vy, vz, fx, fy, fz, c_ID, c_ID[N], f_ID, f_ID[N], v_name

  ```
  x,y,z,vx,vy,vz,fx,fy,fz = atom attribute (position, velocity, force component)
  c_ID = per-atom or local vector calculated by a compute with ID
  c_ID[I] = Ith column of per-atom or local array calculated by a compute with ID,
  ↪I can include wildcard (see below)
  f_ID = per-atom or local vector calculated by a fix with ID
  f_ID[I] = Ith column of per-atom or local array calculated by a fix with ID, I
  ↪can include wildcard (see below)
  v_name = per-atom vector calculated by an atom-style variable with name
  ```

- zero or more keyword/args pairs may be appended
- keyword = *replace*

  ```
  replace args = vec1 vec2
    vec1 = reduced value from this input vector will be replaced
  ```

```
  vec2 = replace it with vec1[N] where N is index of max/min value from␣
↪vec2
```

17.78.2 Examples

```
compute 1 all reduce sum c_force
compute 1 all reduce/region subbox sum c_force
compute 2 all reduce min c_press[2] f_ave v_myKE
compute 2 all reduce min c_press[*] f_ave v_myKE
compute 3 fluid reduce max c_index[1] c_index[2] c_dist replace 1 3 replace 2␣
↪3
```

17.78.3 Description

Define a calculation that "reduces" one or more vector inputs into scalar values, one per listed input. The inputs can be per-atom or local quantities; they cannot be global quantities. Atom attributes are per-atom quantities, *computes* and *fixes* may generate any of the three kinds of quantities, and *atom-style variables* generate per-atom quantities. See the *variable* command and its special functions which can perform the same operations as the compute reduce command on global vectors.

The reduction operation is specified by the *mode* setting. The *sum* option adds the values in the vector into a global total. The *min* or *max* options find the minimum or maximum value across all vector values. The *ave* setting adds the vector values into a global total, then divides by the number of values in the vector. The *sumsq* option sums the square of the values in the vector into a global total. The *avesq* setting does the same as *sumsq*, then divides the sum of squares by the number of values. The last two options can be useful for calculating the variance of some quantity, e.g. variance = sumsq - ave^2.

Each listed input is operated on independently. For per-atom inputs, the group specified with this command means only atoms within the group contribute to the result. For per-atom inputs, if the compute reduce/region command is used, the atoms must also currently be within the region. Note that an input that produces per-atom quantities may define its own group which affects the quantities it returns. For example, if a compute is used as an input which generates a per-atom vector, it will generate values of 0.0 for atoms that are not in the group specified for that compute.

Each listed input can be an atom attribute (position, velocity, force component) or can be the result of a *compute* or *fix* or the evaluation of an atom-style *variable*.

Note that for values from a compute or fix, the bracketed index I can be specified using a wildcard asterisk with the index to effectively specify multiple values. This takes the form "*" or "*n" or "n*" or "m*n". If N = the size of the vector (for *mode* = scalar) or the number of columns in the array (for *mode* = vector), then an asterisk with no numeric values means all indices from 1 to N. A leading asterisk means all indices from 1 to n (inclusive). A trailing asterisk means all indices from n to N (inclusive). A middle asterisk means all indices from m to n (inclusive).

Using a wildcard is the same as if the individual columns of the array had been listed one by one. E.g. these 2 compute reduce commands are equivalent, since the *compute stress/atom* command creates a per-atom array with 6 columns:

```
compute myPress all stress/atom NULL
compute 2 all reduce min c_myPress[*]
compute 2 all reduce min c_myPress[1] c_myPress[2] c_myPress[3] &
                         c_myPress[4] c_myPress[5] c_myPress[6]
```

The atom attribute values (x,y,z,vx,vy,vz,fx,fy,fz) are self-explanatory. Note that other atom attributes can be used as inputs to this fix by using the *compute property/atom* command and then specifying an input value from that compute.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. Computes can generate per-atom or local quantities. See the individual *compute* doc page for details. If no bracketed integer is

appended, the vector calculated by the compute is used. If a bracketed integer is appended, the Ith column of the array calculated by the compute is used. Users can also write code for their own compute styles and *add them to LAMMPS*. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. Fixes can generate per-atom or local quantities. See the individual *fix* doc page for details. Note that some fixes only produce their values on certain timesteps, which must be compatible with when compute reduce references the values, else an error results. If no bracketed integer is appended, the vector calculated by the fix is used. If a bracketed integer is appended, the Ith column of the array calculated by the fix is used. Users can also write code for their own fix style and *add them to LAMMPS*. See the discussion above for how I can be specified with a wildcard asterisk to effectively specify multiple values.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. It must be an *atom-style variable*. Atom-style variables can reference thermodynamic keywords and various per-atom attributes, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of generating per-atom quantities to reduce.

If the *replace* keyword is used, two indices *vec1* and *vec2* are specified, where each index ranges from 1 to the # of input values. The replace keyword can only be used if the *mode* is *min* or *max*. It works as follows. A min/max is computed as usual on the *vec2* input vector. The index N of that value within *vec2* is also stored. Then, instead of performing a min/max on the *vec1* input vector, the stored index is used to select the Nth element of the *vec1* vector.

Thus, for example, if you wish to use this compute to find the bond with maximum stretch, you can do it as follows:

```
compute 1 all property/local batom1 batom2
compute 2 all bond/local dist
compute 3 all reduce max c_1[1] c_1[2] c_2 replace 1 3 replace 2 3
thermo_style custom step temp c_3[1] c_3[2] c_3[3]
```

The first two input values in the compute reduce command are vectors with the IDs of the 2 atoms in each bond, using the *compute property/local* command. The last input value is bond distance, using the *compute bond/local* command. Instead of taking the max of the two atom ID vectors, which does not yield useful information in this context, the *replace* keywords will extract the atom IDs for the two atoms in the bond of maximum stretch. These atom IDs and the bond stretch will be printed with thermodynamic output.

If a single input is specified this compute produces a global scalar value. If multiple inputs are specified, this compute produces a global vector of values, the length of which is equal to the number of inputs specified.

As discussed below, for the *sum* and *sumsq* modes, the value(s) produced by this compute are all "extensive", meaning their value scales linearly with the number of atoms involved. If normalized values are desired, this compute can be accessed by the *thermo_style custom* command with *thermo_modify norm yes* set as an option. Or it can be accessed by a *variable* that divides by the appropriate atom count.

Output info:

This compute calculates a global scalar if a single input value is specified or a global vector of length N where N is the number of inputs, and which can be accessed by indices 1 to N. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

All the scalar or vector values calculated by this compute are "intensive", except when the *sum* or *sumsq* modes are used on per-atom or local vectors, in which case the calculated values are "extensive".

The scalar or vector values will be in whatever *units* the quantities being reduced are in.

17.78.4 Restrictions

none

17.78.5 Related commands

compute, *fix*, *variable*

Default: none

17.79 compute reduce/chunk command

17.79.1 Syntax

```
compute ID group-ID reduce/chunk chunkID mode input1 input2 ...
```

- ID, group-ID are documented in *compute* command
- reduce/chunk = style name of this compute command
- chunkID = ID of *compute chunk/atom* command
- mode = *sum* or *min* or *max*
- one or more inputs can be listed
- input = c_ID, c_ID[N], f_ID, f_ID[N], v_ID

```
c_ID = per-atom vector calculated by a compute with ID
c_ID[I] = Ith column of per-atom array calculated by a compute with ID, I can␣
↪include wildcard (see below)
f_ID = per-atom vector calculated by a fix with ID
f_ID[I] = Ith column of per-atom array calculated by a fix with ID, I can include␣
↪wildcard (see below)
v_name = per-atom vector calculated by an atom-style variable with name
```

17.79.2 Examples

```
compute 1 all reduce/chunk/atom mychunk min c_cluster
```

17.79.3 Description

Define a calculation that reduces one or more per-atom vectors into per-chunk values. This can be useful for diagnostic output. Or when used in conjunction with the *compute chunk/spread/atom* command it can be used ot create per-atom values that induce a new set of chunks with a second *compute chunk/atom* command. An example is given below.

In LAMMPS, chunks are collections of atoms defined by a *compute chunk/atom* command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the *compute chunk/atom* and *Howto chunk* doc pages for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

For each atom, this compute accesses its chunk ID from the specified *chunkID* compute. The per-atom value from an input contributes to a per-chunk value corresponding the the chunk ID.

The reduction operation is specified by the *mode* setting and is performed over all the per-atom values from the atoms in each chunk. The *sum* option adds the pre-atom values to a per-chunk total. The *min* or *max* options find the minimum or maximum value of the per-atom values for each chunk.

Note that only atoms in the specified group contribute to the reduction operation. If the *chunkID* compute returns a 0 for the chunk ID of an atom (i.e. the atom is not in a chunk defined by the *compute chunk/atom* command), that atom will also not contribute to the reduction operation. An input that is a compute or fix may define its own group which affects the quantities it returns. For example, a compute with return a zero value for atoms that are not in the group specified for that compute.

Each listed input is operated on independently. Each input can be the result of a *compute* or *fix* or the evaluation of an atom-style *variable*.

Note that for values from a compute or fix, the bracketed index I can be specified using a wildcard asterisk with the index to effectively specify multiple values. This takes the form "*" or "*n" or "n*" or "m*n". If N = the size of the vector (for *mode* = scalar) or the number of columns in the array (for *mode* = vector), then an asterisk with no numeric values means all indices from 1 to N. A leading asterisk means all indices from 1 to n (inclusive). A trailing asterisk means all indices from n to N (inclusive). A middle asterisk means all indices from m to n (inclusive).

Using a wildcard is the same as if the individual columns of the array had been listed one by one. E.g. these 2 compute reduce/chunk commands are equivalent, since the *compute property/chunk* command creates a per-atom array with 3 columns:

```
compute prop all property/atom vx vy vz
compute 10 all reduce/chunk mychunk max c_prop[*]
compute 10 all reduce/chunk mychunk max c_prop[1] c_prop[2] c_prop[3]
```

Here is an example of using this compute, in conjunction with the compute chunk/spread/atom command to identify self-assembled micelles. The commands below can be added to the examples/in.micelle script.

Imagine a collection of polymer chains or small molecules with hydrophobic end groups. All the hydrophobic (HP) atoms are assigned to a group called "phobic".

These commands will assign a unique cluster ID to all HP atoms within a specified distance of each other. A cluster will contain all HP atoms in a single molecule, but also the HP atoms in nearby molecules, e.g. molecules that have clumped to form a micelle due to the attraction induced by the hydrophobicity. The output of the chunk/reduce command will be a cluster ID per chunk (molecule). Molecules with the same cluster ID are in the same micelle.

```
group phobic type 4     # specific to in.micelle model
compute cluster phobic cluster/atom 2.0
compute cmol all chunk/atom molecule
compute reduce phobic reduce/chunk cmol min c_cluster
```

This per-chunk info could be output in at least two ways:

```
fix 10 all ave/time 1000 1 1000 c_reduce file tmp.phobic mode vector

compute spread all chunk/spread/atom cmol c_reduce
dump 1 all custom 1000 tmp.dump id type mol x y z c_cluster c_spread
dump_modify 1 sort id
```

In the first case, each snapshot in the tmp.phobic file will contain one line per molecule. Molecules with the same value are in the same micelle. In the second case each dump snapshot contains all atoms, each with a final field with the cluster ID of the micelle that the HP atoms of that atom's molecule belong to.

The result from compute chunk/spread/atom can be used to define a new set of chunks, where all the atoms in all the molecules in the same micelle are assigned to the same chunk, i.e. one chunk per micelle.

```
compute micelle all chunk/atom c_spread compress yes
```

Further analysis on a per-micelle basis can now be performed using any of the per-chunk computes listed on the *Howto chunk* doc page. E.g. count the number of atoms in each micelle, calculate its center or mass, shape (moments of inertia), radius of gyration, etc.

```
compute prop all property/chunk micelle count
fix 20 all ave/time 1000 1 1000 c_prop file tmp.micelle mode vector
```

Each snapshot in the tmp.micelle file will have one line per micelle with its count of atoms, plus a first line for a chunk with all the solvent atoms. By the time 50000 steps have elapsed there are a handful of large micelles.

Output info:

This compute calculates a global vector if a single input value is specified, otherwise a global array is output. The number of columns in the array is the number of inputs provided. The length of the vector or the number of vector elements or array rows = the number of chunks *Nchunk* as calculated by the specified *compute chunk/atom* command. The vector or array can be accessed by any command that uses global values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom values for the vector or each column of the array will be in whatever *units* the corresponding input value is in. The vector or array values are "intensive".

17.79.4 Restrictions

none

17.79.5 Related commands

compute chunk/atom, *compute reduce*, *compute chunk/spread/atom*

Default: none

17.80 compute rigid/local command

17.80.1 Syntax

```
compute ID group-ID rigid/local rigidID input1 input2 ...
```

- ID, group-ID are documented in *compute* command
- rigid/local = style name of this compute command
- rigidID = ID of fix rigid/small command or one of its variants
- input = one or more rigid body attributes

```
possible attributes = id, mol, mass,
                      x, y, z, xu, yu, zu, ix, iy, iz
                      vx, vy, vz, fx, fy, fz,
                      omegax, omegay, omegaz,
                      angmomx, angmomy, angmomz,
```

```
                    quatw, quati, quatj, quatk,
                    tqx, tqy, tqz,
                    inertiax, inertiay, inertiaz
id = atom ID of atom within body which owns body properties
mol = molecule ID used to define body in fix rigid/small command
mass = total mass of body
x,y,z = center of mass coords of body
xu,yu,zu = unwrapped center of mass coords of body
ix,iy,iz = box image that the center of mass is in
vx,vy,vz = center of mass velocities
fx,fy,fz = force of center of mass
omegax,omegay,omegaz = angular velocity of body
angmomx,angmomy,angmomz = angular momentum of body
quatw,quati,quatj,quatk = quaternion components for body
tqx,tqy,tqz = torque on body
inertiax,inertiay,inertiaz = diagonalized moments of inertia of body
```

17.80.2 Examples

```
compute 1 all rigid/local myRigid mol x y z
```

17.80.3 Description

Define a computation that simply stores rigid body attributes for rigid bodies defined by the *fix rigid/small* command or one of its NVE, NVT, NPT, NPH variants. The data is stored as local data so it can be accessed by other *output commands* that process local data, such as the *compute reduce* or *dump local* commands.

Note that this command only works with the *fix rigid/small* command or its variants, not the fix rigid command and its variants. The ID of the *fix rigid/small* command used to define rigid bodies must be specified as *rigidID*. The *fix rigid* command is typically used to define a handful of (potentially very large) rigid bodies. It outputs similar per-body information as this command directly from the fix as global data; see the *fix rigid* doc page for details

The local data stored by this command is generated by looping over all the atoms owned on a processor. If the atom is not in the specified *group-ID* or is not part of a rigid body it is skipped. If it is not the atom within a body that is assigned to store the body information it is skipped (only one atom per body is so assigned). If it is the assigned atom, then the info for that body is output. This means that information for N bodies is generated. N may be less than the # of bodies defined by the fix rigid command, if the atoms in some bodies are not in the *group-ID*.

Note: Which atom in a body owns the body info is determined internal to LAMMPS; it's the one nearest the geometric center of the body. Typically you should avoid this complication, by defining the group associated with this fix to include/exclude entire bodies.

Note that as atoms and bodies migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next.

Here is an example of how to use this compute to dump rigid body info to a file:

```
compute 1 all rigid/local myRigid mol x y z fx fy fz
dump 1 all local 1000 tmp.dump index c_1[1] c_1[2] c_1[3] c_1[4] c_1[5] c_1[6] c_1[7]
```

This section explains the rigid body attributes that can be specified.

The *id* attribute is the atom-ID of the atom which owns the rigid body, which is assigned by the *fix rigid/small* command.

The *mol* attribute is the molecule ID of the rigid body. It should be the molecule ID which all of the atoms in the body belong to, since that is how the *fix rigid/small* command defines its rigid bodies.

The *mass* attribute is the total mass of the rigid body.

There are two options for outputting the coordinates of the center of mass (COM) of the body. The *x*, *y*, *z* attributes write the COM "unscaled", in the appropriate distance *units* (Angstroms, sigma, etc). Use *xu*, *yu*, *zu* if you want the COM "unwrapped" by the image flags for each body. Unwrapped means that if the body COM has passed through a periodic boundary one or more times, the value is generated what the COM coordinate would be if it had not been wrapped back into the periodic box.

The image flags for the body can be generated directly using the *ix*, *iy*, *iz* attributes. For periodic dimensions, they specify which image of the simulation box the COM is considered to be in. An image of 0 means it is inside the box as defined. A value of 2 means add 2 box lengths to get the true value. A value of -1 means subtract 1 box length to get the true value. LAMMPS updates these flags as the rigid body COMs cross periodic boundaries during the simulation.

The *vx*, *vy*, *vz*, *fx*, *fy*, *fz* attributes are components of the COM velocity and force on the COM of the body.

The *omegax*, *omegay*, and *omegaz* attributes are the angular velocity components of the body around its COM.

The *angmomx*, *angmomy*, and *angmomz* attributes are the angular momentum components of the body around its COM.

The *quatw*, *quati*, *quatj*, and *quatk* attributes are the components of the 4-vector quaternion representing the orientation of the rigid body. See the *set* command for an explanation of the quaternion vector.

The *angmomx*, *angmomy*, and *angmomz* attributes are the angular momentum components of the body around its COM.

The *tqx*, *tqy*, *tqz* attributes are components of the torque acting on the body around its COM.

The *inertiax*, *inertiay*, *inertiaz* attributes are components of diagonalized inertia tensor for the body, i.e the 3 moments of inertia for the body around its principal axes, as computed internally by LAMMPS.

Output info:

This compute calculates a local vector or local array depending on the number of keywords. The length of the vector or number of rows in the array is the number of rigid bodies. If a single keyword is specified, a local vector is produced. If two or more keywords are specified, a local array is produced where the number of columns = the number of keywords. The vector or array can be accessed by any command that uses local values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector or array values will be in whatever *units* the corresponding attribute is in:

- id,mol = unitless
- mass = mass units
- x,y,z and xy,yu,zu = distance units
- vx,vy,vz = velocity units
- fx,fy,fz = force units
- omegax,omegay,omegaz = radians/time units
- angmomx,angmomy,angmomz = mass*distance^2/time units
- quatw,quati,quatj,quatk = unitless
- tqx,tqy,tqz = torque units

- inertiax,inertiay,inertiaz = mass*distance^2 units

17.80.4 Restrictions

This compute is part of the RIGID package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.80.5 Related commands

dump local, *compute reduce*

Default: none

17.81 compute saed command

17.81.1 Syntax

```
compute ID group-ID saed lambda type1 type2 ... typeN keyword value ...
```

- ID, group-ID are documented in *compute* command
- saed = style name of this compute command
- lambda = wavelength of incident radiation (length units)
- type1 type2 ... typeN = chemical symbol of each atom type (see valid options below)
- zero or more keyword/value pairs may be appended
- keyword = *Kmax* or *Zone* or *dR_Ewald* or *c* or *manual* or *echo*

```
Kmax value = Maximum distance explored from reciprocal space origin
               (inverse length units)
Zone values = z1 z2 z3
  z1,z2,z3 = Zone axis of incident radiation. If z1=z2=z3=0 all
             reciprocal space will be meshed up to Kmax
dR_Ewald value = Thickness of Ewald sphere slice intercepting
                  reciprocal space (inverse length units)
c values = c1 c2 c3
  c1,c2,c3 = parameters to adjust the spacing of the reciprocal
             lattice nodes in the h, k, and l directions respectively
manual = flag to use manual spacing of reciprocal lattice points
           based on the values of the c parameters
echo = flag to provide extra output for debugging purposes
```

17.81.2 Examples

```
compute 1 all saed 0.0251 Al O Kmax 1.70 Zone 0 0 1 dR_Ewald 0.01 c 0.5 0.5 0.5
compute 2 all saed 0.0251 Ni Kmax 1.70 Zone 0 0 0 c 0.05 0.05 0.05 manual echo

fix saed/vtk 1 1 1 c_1 file Al2O3_001.saed
fix saed/vtk 1 1 1 c_2 file Ni_000.saed
```

17.81.3 Description

Define a computation that calculates electron diffraction intensity as described in *(Coleman)* on a mesh of reciprocal lattice nodes defined by the entire simulation domain (or manually) using simulated radiation of wavelength lambda.

The electron diffraction intensity I at each reciprocal lattice point is computed from the structure factor F using the equations:

$$I = \frac{F^* F}{N}$$
$$F(\mathbf{k}) = \sum_{j=1}^{N} f_j(\theta) exp(2\pi i \mathbf{k} \cdot \mathbf{r}_j)$$

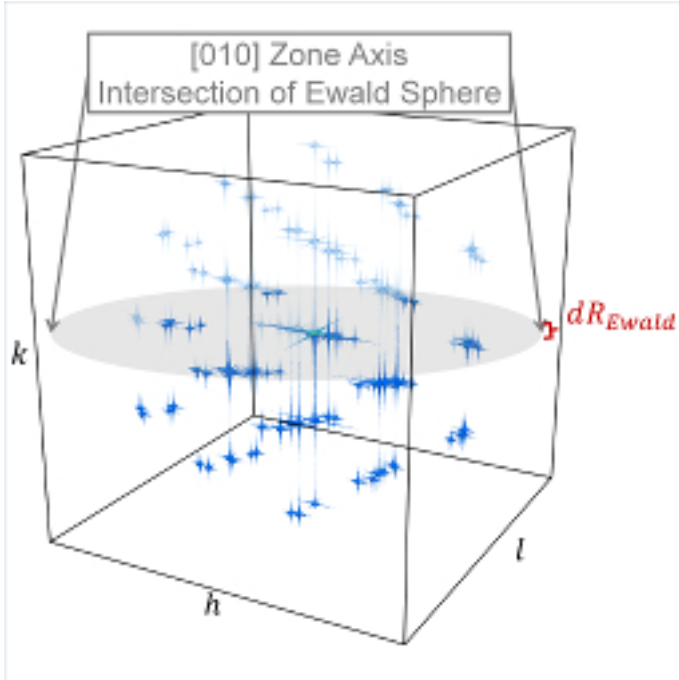
Here, K is the location of the reciprocal lattice node, r_j is the position of each atom, f_j are atomic scattering factors.

Diffraction intensities are calculated on a three-dimensional mesh of reciprocal lattice nodes. The mesh spacing is defined either (a) by the entire simulation domain or (b) manually using selected values as shown in the 2D diagram below.

For a mesh defined by the simulation domain, a rectilinear grid is constructed with spacing *c**inv(A) along each reciprocal lattice axis. Where A are the vectors corresponding to the edges of the simulation cell. If one or two directions has non-periodic boundary conditions, then the spacing in these directions is defined from the average of the (inversed) box lengths with periodic boundary conditions. Meshes defined by the simulation domain must contain at least one periodic boundary.

If the *manual* flag is included, the mesh of reciprocal lattice nodes will defined using the *c* values for the spacing along each reciprocal lattice axis. Note that manual mapping of the reciprocal space mesh is good for comparing diffraction results from multiple simulations; however it can reduce the likelihood that Bragg reflections will be satisfied unless small spacing parameters <0.05 Angstrom^(-1) are implemented. Meshes with manual spacing do not require a periodic boundary.

The limits of the reciprocal lattice mesh are determined by the use of the *Kmax*, *Zone*, and *dR_Ewald* parameters. The rectilinear mesh created about the origin of reciprocal space is terminated at the boundary of a sphere of radius *Kmax* centered at the origin. If *Zone* parameters z1=z2=z3=0 are used, diffraction intensities are computed throughout the entire spherical volume - note this can greatly increase the cost of computation. Otherwise, *Zone* parameters will denote the z1=h, z2=k, and z3=l (in a global since) zone axis of an intersecting Ewald sphere. Diffraction intensities will only be computed at the intersection of the reciprocal lattice mesh and a *dR_Ewald* thick surface of the Ewald sphere. See the example 3D intensity data and the intersection of a [010] zone axis in the below image.



The atomic scattering factors, fj, accounts for the reduction in diffraction intensity due to Compton scattering. Compute saed uses analytical approximations of the atomic scattering factors that vary for each atom type (type1 type2 . . . typeN) and angle of diffraction. The analytic approximation is computed using the formula *(Brown)*:

$$f_j\left(\frac{sin(\theta)}{\lambda}\right) = \sum_i^5 a_i exp\left(-b_i \frac{sin^2(\theta)}{\lambda^2}\right)$$

Coefficients parameterized by *(Fox)* are assigned for each atom type designating the chemical symbol and charge of each atom type. Valid chemical symbols for compute saed are:

H	He	Li	Be	B	C	N	O	F	Ne	Na	Mg	Al	Si	P	S	Cl	Ar	K	Ca
Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	Rb	Sr	Y	Zr
Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	Cs	Ba	La	Ce	Pr	Nd
Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg
Tl	Pb	Bi	Po	At	Rn	Fr	Ra	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf		

If the *echo* keyword is specified, compute saed will provide extra reporting information to the screen.

Output info:

This compute calculates a global vector. The length of the vector is the number of reciprocal lattice nodes that are explored by the mesh. The entries of the global vector are the computed diffraction intensities as described above.

The vector can be accessed by any command that uses global values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

All array values calculated by this compute are "intensive".

17.81.4 Restrictions

This compute is part of the USER-DIFFRACTION package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

The compute_saed command does not work for triclinic cells.

17.81.5 Related commands

fix saed_vtk, *compute xrd*

17.81.6 Default

The option defaults are Kmax = 1.70, Zone 1 0 0, c 1 1 1, dR_Ewald = 0.01.

(Coleman) Coleman, Spearot, Capolungo, MSMSE, 21, 055020 (2013).

(Brown) Brown et al. International Tables for Crystallography Volume C: Mathematical and Chemical Tables, 554-95 (2004).

(Fox) Fox, O'Keefe, Tabbernor, Acta Crystallogr. A, 45, 786-93 (1989).

17.82 compute slice command

17.82.1 Syntax

```
compute ID group-ID slice Nstart Nstop Nskip input1 input2 ...
```

- ID, group-ID are documented in *compute* command
- slice = style name of this compute command
- Nstart = starting index within input vector(s)
- Nstop = stopping index within input vector(s)
- Nskip = extract every Nskip elements from input vector(s)
- input = c_ID, c_ID[N], f_ID, f_ID[N]

```
c_ID = global vector calculated by a compute with ID
c_ID[I] = Ith column of global array calculated by a compute with ID
f_ID = global vector calculated by a fix with ID
f_ID[I] = Ith column of global array calculated by a fix with ID
v_name = vector calculated by an vector-style variable with name
```

17.82.2 Examples

```
compute 1 all slice 1 100 10 c_msdmol[4]
compute 1 all slice 301 400 1 c_msdmol[4] v_myVec
```

17.82.3 Description

Define a calculation that "slices" one or more vector inputs into smaller vectors, one per listed input. The inputs can be global quantities; they cannot be per-atom or local quantities. *Computes* and *fixes* and vector-style *variables* can generate such global quantities. The group specified with this command is ignored.

The values extracted from the input vector(s) are determined by the *Nstart*, *Nstop*, and *Nskip* parameters. The elements of an input vector of length N are indexed from 1 to N. Starting at element *Nstart*, every Mth element is extracted, where M = *Nskip*, until element *Nstop* is reached. The extracted quantities are stored as a vector, which is typically shorter than the input vector.

Each listed input is operated on independently to produce one output vector. Each listed input must be a global vector or column of a global array calculated by another *compute* or *fix*.

If an input value begins with "c_", a compute ID must follow which has been previously defined in the input script and which generates a global vector or array. See the individual *compute* doc page for details. If no bracketed integer is appended, the vector calculated by the compute is used. If a bracketed integer is appended, the Ith column of the array calculated by the compute is used. Users can also write code for their own compute styles and *add them to LAMMPS*.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script and which generates a global vector or array. See the individual *fix* doc page for details. Note that some fixes only produce their values on certain timesteps, which must be compatible with when compute slice references the values, else an error results. If no bracketed integer is appended, the vector calculated by the fix is used. If a bracketed integer is appended, the Ith column of the array calculated by the fix is used. Users can also write code for their own fix style and *add them to LAMMPS*.

If an input value begins with "v_", a variable name must follow which has been previously defined in the input script. Only vector-style variables can be referenced. See the *variable* command for details. Note that variables of style *vector* define a formula which can reference individual atom properties or thermodynamic keywords, or they can invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of specifying quantities to slice.

If a single input is specified this compute produces a global vector, even if the length of the vector is 1. If multiple inputs are specified, then a global array of values is produced, with the number of columns equal to the number of inputs specified.

Output info:

This compute calculates a global vector if a single input value is specified or a global array with N columns where N is the number of inputs. The length of the vector or the number of rows in the array is equal to the number of values extracted from each input vector. These values can be used by any command that uses global vector or array values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector or array values calculated by this compute are simply copies of values generated by computes or fixes or variables that are input vectors to this compute. If there is a single input vector of intensive and/or extensive values, then each value in the vector of values calculated by this compute will be "intensive" or "extensive", depending on the corresponding input value. If there are multiple input vectors, and all the values in them are intensive, then the array values calculated by this compute are "intensive". If there are multiple input vectors, and any value in them is extensive, then the array values calculated by this compute are "extensive". Values produced by a variable are treated as intensive.

The vector or array values will be in whatever *units* the input quantities are in.

17.82.4 Restrictions

none

17.82.5 Related commands

compute, *fix*, *compute reduce*

Default: none

17.83 compute smd/contact/radius command

17.83.1 Syntax

```
compute ID group-ID smd/contact/radius
```

- ID, group-ID are documented in *compute* command
- smd/contact/radius = style name of this compute command

17.83.2 Examples

```
compute 1 all smd/contact/radius
```

17.83.3 Description

Define a computation which outputs the contact radius, i.e., the radius used to prevent particles from penetrating each other. The contact radius is used only to prevent particles belonging to different physical bodies from penetrating each other. It is used by the contact pair styles, e.g., smd/hertz and smd/tri_surface.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

The value of the contact radius will be 0.0 for particles not in the specified compute group.

Output info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-particle vector values will be in distance *units*.

17.83.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.83.5 Related commands

dump custom smd/hertz smd/tri_surface

Default: none

17.84 compute smd/damage command

17.84.1 Syntax

```
compute ID group-ID smd/damage
```

- ID, group-ID are documented in *compute* command
- smd/damage = style name of this compute command

17.84.2 Examples

```
compute 1 all smd/damage
```

17.84.3 Description

Define a computation that calculates the damage status of SPH particles according to the damage model which is defined via the SMD SPH pair styles, e.g., the maximum plastic strain failure criterion.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Output Info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-particle values are dimensionless an in the range of zero to one.

17.84.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the "Build

17.84.5 Related commands

smd/plastic_strain, *smd/tlsph_stress*

Default: none

17.85 compute smd/hourglass/error command

17.85.1 Syntax

```
compute ID group-ID smd/hourglass/error
```

- ID, group-ID are documented in *compute* command
- smd/hourglass/error = style name of this compute command

17.85.2 Examples

```
compute 1 all smd/hourglass/error
```

17.85.3 Description

Define a computation which outputs the error of the approximated relative separation with respect to the actual relative separation of the particles i and j. Ideally, if the deformation gradient is exact, and there exists a unique mapping between all particles' positions within the neighborhood of the central node and the deformation gradient, the approximated relative separation will coincide with the actual relative separation of the particles i and j in the deformed configuration. This compute is only really useful for debugging the hourglass control mechanism which is part of the Total-Lagrangian SPH pair style.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Output Info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-particle vector values will are dimensionless. See *units*.

17.85.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This quantity will be computed only for particles which interact with tlsph pair style.

Related Commands:

smd/tlsph_defgrad

17.85.5 Default

17.86 compute smd/internal/energy command

17.86.1 Syntax

```
compute ID group-ID smd/internal/energy
```

- ID, group-ID are documented in *compute* command
- smd/smd/internal/energy = style name of this compute command

17.86.2 Examples

```
compute 1 all smd/internal/energy
```

17.86.3 Description

Define a computation which outputs the per-particle enthalpy, i.e., the sum of potential energy and heat.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Output Info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-particle vector values will be given in *units* of energy.

17.86.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info. This compute can only be used for particles which interact via the updated Lagrangian or total Lagrangian SPH pair styles.

Related Commands:

17.86.5 Default

17.87 compute smd/plastic/strain command

17.87.1 Syntax

```
compute ID group-ID smd/plastic/strain
```

- ID, group-ID are documented in *compute* command
- smd/plastic/strain = style name of this compute command

17.87.2 Examples

```
compute 1 all smd/plastic/strain
```

17.87.3 Description

Define a computation that outputs the equivalent plastic strain per particle. This command is only meaningful if a material model with plasticity is defined.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Output Info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-particle values will be given dimensionless. See *units*.

17.87.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info. This compute can only be used for particles which interact via the updated Lagrangian or total Lagrangian SPH pair styles.

17.87.5 Related commands

smd/plastic/strain/rate, *smd/tlsph/strain/rate*, *smd/tlsph/strain*

Default: none

17.88 compute smd/plastic/strain/rate command

17.88.1 Syntax

```
compute ID group-ID smd/plastic/strain/rate
```

- ID, group-ID are documented in *compute* command
- smd/plastic/strain/rate = style name of this compute command

17.88.2 Examples

```
compute 1 all smd/plastic/strain/rate
```

17.88.3 Description

Define a computation that outputs the time rate of the equivalent plastic strain. This command is only meaningful if a material model with plasticity is defined.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Output Info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-particle values will be given in *units* of one over time.

17.88.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info. This compute can only be used for particles which interact via the updated Lagrangian or total Lagrangian SPH pair styles.

17.88.5 Related commands

smd/plastic/strain, *smd/tlsph/strain/rate*, *smd/tlsph/strain*

Default: none

17.89 compute smd/rho command

17.89.1 Syntax

```
compute ID group-ID smd/rho
```

- ID, group-ID are documented in *compute* command
- smd/rho = style name of this compute command

17.89.2 Examples

```
compute 1 all smd/rho
```

17.89.3 Description

Define a computation that calculates the per-particle mass density. The mass density is the mass of a particle which is constant during the course of a simulation, divided by its volume, which can change due to mechanical deformation.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-particle values will be in *units* of mass over volume.

17.89.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.89.5 Related commands

compute smd/vol

Default: none

17.90 compute smd/tlsph/defgrad command

17.90.1 Syntax

```
compute ID group-ID smd/tlsph/defgrad
```

- ID, group-ID are documented in *compute* command
- smd/tlsph/defgrad = style name of this compute command

17.90.2 Examples

```
compute 1 all smd/tlsph/defgrad
```

17.90.3 Description

Define a computation that calculates the deformation gradient. It is only meaningful for particles which interact according to the Total-Lagrangian SPH pair style.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Output info:

This compute outputs a per-particle vector of vectors (tensors), which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-particle vector values will be given dimensionless. See *units*. The per-particle vector has 10 entries. The first nine entries correspond to the xx, xy, xz, yx, yy, yz, zx, zy, zz components of the asymmetric deformation gradient tensor. The tenth entry is the determinant of the deformation gradient.

17.90.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info. TThis compute can only be used for particles which interact via the total Lagrangian SPH pair style.

17.90.5 Related commands

smd/hourglass/error

Default: none

17.91 compute smd/tlsph/dt command

17.91.1 Syntax

```
compute ID group-ID smd/tlsph/dt
```

- ID, group-ID are documented in *compute* command
- smd/tlsph/dt = style name of this compute command

17.91.2 Examples

```
compute 1 all smd/tlsph/dt
```

17.91.3 Description

Define a computation that outputs the CFL-stable time increment per particle. This time increment is essentially given by the speed of sound, divided by the SPH smoothing length. Because both the speed of sound and the smoothing length typically change during the course of a simulation, the stable time increment needs to be re-computed every time step. This calculation is performed automatically in the relevant SPH pair styles and this compute only serves to make the stable time increment accessible for output purposes.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-particle values will be given in *units* of time.

17.91.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This compute can only be used for particles interacting with the Total-Lagrangian SPH pair style.

17.91.5 Related commands

smd/adjust/dt

Default: none

17.92 compute smd/tlsph/num/neighs command

17.92.1 Syntax

```
compute ID group-ID smd/tlsph/num/neighs
```

- ID, group-ID are documented in *compute* command
- smd/tlsph/num/neighs = style name of this compute command

17.92.2 Examples

```
compute 1 all smd/tlsph/num/neighs
```

17.92.3 Description

Define a computation that calculates the number of particles inside of the smoothing kernel radius for particles interacting via the Total-Lagrangian SPH pair style.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-particle values are dimensionless. See *units*.

17.92.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This quantity will be computed only for particles which interact with the Total-Lagrangian pair style.

17.92.5 Related commands

smd/ulsph/num/neighs

Default: none

17.93 compute smd/tlsph/shape command

17.93.1 Syntax

```
compute ID group-ID smd/tlsph/shape
```

- ID, group-ID are documented in *compute* command
- smd/tlsph/shape = style name of this compute command

17.93.2 Examples

```
compute 1 all smd/tlsph/shape
```

17.93.3 Description

Define a computation that outputs the current shape of the volume associated with a particle as a rotated ellipsoid. It is only meaningful for particles which interact according to the Total-Lagrangian SPH pair style.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector of vectors, which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-particle vector has 7 entries. The first three entries correspond to the lengths of the ellipsoid's axes and have units of length. These axis values are computed as the contact radius times the xx, yy, or zz components of the Green-Lagrange strain tensor associated with the particle. The next 4 values are quaternions (order: q, x, y, z) which describe the spatial rotation of the particle relative to its initial state.

17.93.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This quantity will be computed only for particles which interact with the Total-Lagrangian SPH pair style.

17.93.5 Related commands

smd/contact/radius

Default: none

17.94 compute smd/tlsph/strain command

17.94.1 Syntax

```
compute ID group-ID smd/tlsph/strain
```

- ID, group-ID are documented in *compute* command
- smd/tlsph/strain = style name of this compute command

17.94.2 Examples

```
compute 1 all smd/tlsph/strain
```

17.94.3 Description

Define a computation that calculates the Green-Lagrange strain tensor for particles interacting via the Total-Lagrangian SPH pair style.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector of vectors (tensors), which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-particle tensor values will be given dimensionless. See *units*.

The per-particle vector has 6 entries, corresponding to the xx, yy, zz, xy, xz, yz components of the symmetric strain tensor.

17.94.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This quantity will be computed only for particles which interact with the Total-Lagrangian SPH pair style.

17.94.5 Related commands

smd/tlsph/strain/rate, *smd/tlsph/stress*

Default: none

17.95 compute smd/tlsph/strain/rate command

17.95.1 Syntax

```
compute ID group-ID smd/tlsph/strain/rate
```

- ID, group-ID are documented in *compute* command
- smd/tlsph/strain/rate = style name of this compute command

17.95.2 Examples

```
compute 1 all smd/tlsph/strain/rate
```

17.95.3 Description

Define a computation that calculates the rate of the strain tensor for particles interacting via the Total-Lagrangian SPH pair style.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector of vectors (tensors), which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The values will be given in *units* of one over time.

The per-particle vector has 6 entries, corresponding to the xx, yy, zz, xy, xz, yz components of the symmetric strain rate tensor.

17.95.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This quantity will be computed only for particles which interact with Total-Lagrangian SPH pair style.

17.95.5 Related commands

compute smd/tlsph/strain, *compute smd/tlsph/stress*

Default: none

17.96 compute smd/tlsph/stress command

17.96.1 Syntax

```
compute ID group-ID smd/tlsph/stress
```

- ID, group-ID are documented in *compute* command
- smd/tlsph/stress = style name of this compute command

17.96.2 Examples

```
compute 1 all smd/tlsph/stress
```

17.96.3 Description

Define a computation that outputs the Cauchy stress tensor for particles interacting via the Total-Lagrangian SPH pair style.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector of vectors (tensors), which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The values will be given in *units* of pressure.

The per-particle vector has 7 entries. The first six entries correspond to the xx, yy, zz, xy, xz and yz components of the symmetric Cauchy stress tensor. The seventh entry is the second invariant of the stress tensor, i.e., the von Mises equivalent stress.

17.96.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This quantity will be computed only for particles which interact with the Total-Lagrangian SPH pair style.

17.96.5 Related commands

compute smd/tlsph/strain, *cmopute smd/tlsph/strain/rate*

Default: none

17.97 compute smd/triangle/vertices command

17.97.1 Syntax

```
compute ID group-ID smd/triangle/vertices
```

- ID, group-ID are documented in *compute* command
- smd/triangle/vertices = style name of this compute command

17.97.2 Examples

```
compute 1 all smd/triangle/mesh/vertices
```

17.97.3 Description

Define a computation that returns the coordinates of the vertices corresponding to the triangle-elements of a mesh created by the *fix smd/wall_surface*.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute returns a per-particle vector of vectors, which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-particle vector has nine entries, (x1/y1/z1), (x2/y2/z2), and (x3/y3/z3) corresponding to the first, second, and third vertex of each triangle.

It is only meaningful to use this compute for a group of particles which is created via the *fix smd/wall_surface* command.

The output of this compute can be used with the dump2vtk_tris tool to generate a VTK representation of the smd/wall_surface mesh for visualization purposes.

The values will be given in *units* of distance.

17.97.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.97.5 Related commands

fix smd/move/tri/surf, *fix smd/wall_surface*

Default: none

17.98 compute smd/ulsph/num/neighs command

17.98.1 Syntax

```
compute ID group-ID smd/ulsph/num/neighs
```

- ID, group-ID are documented in *compute* command
- smd/ulsph/num/neighs = style name of this compute command

17.98.2 Examples

```
compute 1 all smd/ulsph/num/neighs
```

17.98.3 Description

Define a computation that returns the number of neighbor particles inside of the smoothing kernel radius for particles interacting via the updated Lagrangian SPH pair style.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute returns a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-particle values will be given dimensionless, see *units*.

17.98.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info. This compute can only be used for particles which interact with the updated Lagrangian SPH pair style.

17.98.5 Related commands

compute smd/tlsph/num/neighs

Default: none

17.99 compute smd/ulsph/strain command

17.99.1 Syntax

```
compute ID group-ID smd/ulsph/strain
```

- ID, group-ID are documented in *compute* command
- smd/ulsph/strain = style name of this compute command

17.99.2 Examples

```
compute 1 all smd/ulsph/strain
```

17.99.3 Description

Define a computation that outputs the logarithmic strain tensor. for particles interacting via the updated Lagrangian SPH pair style.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle tensor, which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-particle vector has 6 entries, corresponding to the xx, yy, zz, xy, xz, yz components of the symmetric strain rate tensor.

The per-particle tensor values will be given dimensionless, see *units*.

17.99.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info. This compute can only be used for particles which interact with the updated Lagrangian SPH pair style.

17.99.5 Related commands

compute smd/tlsph/strain

Default: none

17.100 compute smd/ulsph/strain/rate command

17.100.1 Syntax

```
compute ID group-ID smd/ulsph/strain/rate
```

- ID, group-ID are documented in *compute* command
- smd/ulsph/strain/rate = style name of this compute command

17.100.2 Examples

```
compute 1 all smd/ulsph/strain/rate
```

17.100.3 Description

Define a computation that outputs the rate of the logarithmic strain tensor for particles interacting via the updated Lagrangian SPH pair style.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector of vectors (tensors), which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The values will be given in *units* of one over time.

The per-particle vector has 6 entries, corresponding to the xx, yy, zz, xy, xz, yz components of the symmetric strain rate tensor.

17.100.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This compute can only be used for particles which interact with the updated Lagrangian SPH pair style.

17.100.5 Related commands

compute smd/tlsph/strain/rate

Default: none

17.101 compute smd/ulsph/stress command

17.101.1 Syntax

```
compute ID group-ID smd/ulsph/stress
```

- ID, group-ID are documented in *compute* command
- smd/ulsph/stress = style name of this compute command

17.101.2 Examples

```
compute 1 all smd/ulsph/stress
```

17.101.3 Description

Define a computation that outputs the Cauchy stress tensor.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector of vectors (tensors), which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The values will be given in *units* of pressure.

The per-particle vector has 7 entries. The first six entries correspond to the xx, yy, zz, xy, xz, yz components of the symmetric Cauchy stress tensor. The seventh entry is the second invariant of the stress tensor, i.e., the von Mises equivalent stress.

17.101.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info. This compute can only be used for particles which interact with the updated Lagrangian SPH pair style.

17.101.5 Related commands

compute smd/ulsph/strain, *compute smd/ulsph/strain/rate compute smd/tlsph/stress*

Default: none

17.102 compute smd/vol command

17.102.1 Syntax

```
compute ID group-ID smd/vol
```

- ID, group-ID are documented in *compute* command
- smd/vol = style name of this compute command

17.102.2 Examples

```
compute 1 all smd/vol
```

17.102.3 Description

Define a computation that provides the per-particle volume and the sum of the per-particle volumes of the group for which the fix is defined.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-particle vector values will be given in *units* of volume.

Additionally, the compute returns a scalar, which is the sum of the per-particle volumes of the group for which the fix is defined.

17.102.4 Restrictions

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.102.5 Related commands

compute smd/rho

Default: none

17.103 compute sna/atom command

17.104 compute snad/atom command

17.105 compute snav/atom command

17.106 compute snap command

17.106.1 Syntax

```
compute ID group-ID sna/atom rcutfac rfac0 twojmax R_1 R_2 ... w_1 w_2 ... keyword␣
↪values ...
compute ID group-ID snad/atom rcutfac rfac0 twojmax R_1 R_2 ... w_1 w_2 ... keyword␣
↪values ...
compute ID group-ID snav/atom rcutfac rfac0 twojmax R_1 R_2 ... w_1 w_2 ... keyword␣
↪values ...
compute ID group-ID snap rcutfac rfac0 twojmax R_1 R_2 ... w_1 w_2 ... keyword values␣
↪...
```

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- ID, group-ID are documented in *compute* command
- sna/atom = style name of this compute command
- rcutfac = scale factor applied to all cutoff radii (positive real)
- rfac0 = parameter in distance to angle conversion (0 < rcutfac < 1)
- twojmax = band limit for bispectrum components (non-negative integer)
- R_1, R_2,... = list of cutoff radii, one for each type (distance units)
- w_1, w_2,... = list of neighbor weights, one for each type
- zero or more keyword/value pairs may be appended
- keyword = *rmin0* or *switchflag* or *bzeroflag* or *quadraticflag*

```
rmin0 value = parameter in distance to angle conversion (distance units)
switchflag value = 0 or 1
   0 = do not use switching function
   1 = use switching function
bzeroflag value = 0 or 1
   0 = do not subtract B0
   1 = subtract B0
quadraticflag value = 0 or 1
   0 = do not generate quadratic terms
   1 = generate quadratic terms
```

17.106.2 Examples

```
compute b all sna/atom 1.4 0.99363 6 2.0 2.4 0.75 1.0 rmin0 0.0
compute db all sna/atom 1.4 0.95 6 2.0 1.0
compute vb all sna/atom 1.4 0.95 6 2.0 1.0
compute snap all snap 1.4 0.95 6 2.0 1.0
```

17.106.3 Description

Define a computation that calculates a set of quantities related to the bispectrum components of the atoms in a group. These computes are used primarily for calculating the dependence of energy, force, and stress components on the linear coefficients in the *snap pair_style*, which is useful when training a SNAP potential to match target data.

Bispectrum components of an atom are order parameters characterizing the radial and angular distribution of neighbor atoms. The detailed mathematical definition is given in the paper by Thompson et al. *(Thompson)*

The position of a neighbor atom *i'* relative to a central atom *i* is a point within the 3D ball of radius *R_ii' = rcutfac*(R_i + R_i')*

Bartok et al. *(Bartok)*, proposed mapping this 3D ball onto the 3-sphere, the surface of the unit ball in a four-dimensional space. The radial distance *r* within *R_ii'* is mapped on to a third polar angle *theta0* defined by,

$$\theta_0 = \texttt{rfac0}\frac{r - r_{min0}}{R_{ii'} - r_{min0}}\pi$$

In this way, all possible neighbor positions are mapped on to a subset of the 3-sphere. Points south of the latitude *theta0max=rfac0*Pi* are excluded.

The natural basis for functions on the 3-sphere is formed by the 4D hyperspherical harmonics *U^j_m,m'(theta, phi, theta0)*. These functions are better known as *D^j_m,m'*, the elements of the Wigner *D*-matrices *(Meremianin, Varshalovich)*.

The density of neighbors on the 3-sphere can be written as a sum of Dirac-delta functions, one for each neighbor, weighted by species and radial distance. Expanding this density function as a generalized Fourier series in the basis functions, we can write each Fourier coefficient as

$$u^j_{m,m'} = U^j_{m,m'}(0,0,0) + \sum_{r_{ii'}<R_{ii'}} f_c(r_{ii'}) w_{i'} U^j_{m,m'}(\theta_0,\theta,\phi)$$

The *w_i'* neighbor weights are dimensionless numbers that are chosen to distinguish atoms of different types, while the central atom is arbitrarily assigned a unit weight. The function *fc(r)* ensures that the contribution of each neighbor atom goes smoothly to zero at *R_ii'*:

$$\begin{aligned} f_c(r) =& \frac{1}{2}(\cos(\pi\frac{r-r_{min0}}{R_{ii'}-r_{min0}})+1), r \le R_{ii'} \\ =& 0, r > R_{ii'} \end{aligned}$$

The expansion coefficients *u^j_m,m'* are complex-valued and they are not directly useful as descriptors, because they are not invariant under rotation of the polar coordinate frame. However, the following scalar triple products of expansion coefficients can be shown to be real-valued and invariant under rotation *(Bartok)*.

$$B_{j_1,j_2,j} = \sum_{m_1,m_1'=-j_1}^{j_1} \sum_{m_2,m_2'=-j_2}^{j_2} \sum_{m,m'=-j}^{j} (u^j_{m,m'})^* H \begin{matrix} jmm' \\ j_1 m_1 m_1' \\ j_2 m_2 m_2' \end{matrix} u^{j_1}_{m_1,m_1'} u^{j_2}_{m_2,m_2'}$$

The constants *H^jmm'_j1m1m1'_j2m2m2'* are coupling coefficients, analogous to Clebsch-Gordan coefficients for rotations on the 2-sphere. These invariants are the components of the bispectrum and these are the quantities calculated by the compute *sna/atom*. They characterize the strength of density correlations at three points on the 3-sphere. The j2=0 subset form the power spectrum, which characterizes the correlations of two points. The lowest-order components describe the coarsest features of the density function, while higher-order components reflect finer detail. Note that the central atom is included in the expansion, so three point-correlations can be either due to three neighbors, or two neighbors and the central atom.

Compute *snad/atom* calculates the derivative of the bispectrum components summed separately for each atom type:

$$-\sum_{i'\in I} \frac{\partial B^{i'}_{j_1,j_2,j}}{\partial \mathbf{r}_i}$$

The sum is over all atoms *i'* of atom type *I*. For each atom *i*, this compute evaluates the above expression for each direction, each atom type, and each bispectrum component. See section below on output for a detailed explanation.

Compute *snav/atom* calculates the virial contribution due to the derivatives:

$$-\mathbf{r}_i \otimes \sum_{i'\in I} \frac{\partial B^{i'}_{j_1,j_2,j}}{\partial \mathbf{r}_i}$$

Again, the sum is over all atoms *i'* of atom type *I*. For each atom *i*, this compute evaluates the above expression for each of the six virial components, each atom type, and each bispectrum component. See section below on output for a detailed explanation.

Compute *snap* calculates a global array contains information related to all three of the above per-atom computes *sna/atom*, *snad/atom*, and *snav/atom*. The first row of the array contains the summation of *sna/atom* over all atoms, but broken out by type. The last six rows of the array contain the summation of *snav/atom* over all atoms, broken out by type. In between these are 3**N* rows containing the same values computed by *snad/atom* (these are already summed over all atoms and broken out by type). The element in the last column of each row contains the potential

energy, force, or stress, according to the row. These quantities correspond to the user-specified reference potential that must be subtracted from the target data when fitting SNAP. The potential energy calculation uses the built in compute *thermo_pe*. The stress calculation uses a compute called *snap_press* that is automatically created behind the scenes, according to the following command:

```
compute snap_press all pressure NULL virial
```

See section below on output for a detailed explanation of the data layout in the global array.

The value of all bispectrum components will be zero for atoms not in the group. Neighbor atoms not in the group do not contribute to the bispectrum of atoms in the group.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (i.e. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently.

The argument *rcutfac* is a scale factor that controls the ratio of atomic radius to radial cutoff distance.

The argument *rfac0* and the optional keyword *rmin0* define the linear mapping from radial distance to polar angle *theta0* on the 3-sphere.

The argument *twojmax* defines which bispectrum components are generated. See section below on output for a detailed explanation of the number of bispectrum components and the ordered in which they are listed.

The keyword *switchflag* can be used to turn off the switching function.

The keyword *bzeroflag* determines whether or not *B0*, the bispectrum components of an atom with no neighbors, are subtracted from the calculated bispectrum components. This optional keyword normally only affects compute *sna/atom*. However, when *quadraticflag* is on, it also affects *snad/atom* and *snav/atom*.

The keyword *quadraticflag* determines whether or not the quadratic analogs to the bispectrum quantities are generated. These are formed by taking the outer product of the vector of bispectrum components with itself. See section below on output for a detailed explanation of the number of quadratic terms and the ordered in which they are listed.

Note: If you have a bonded system, then the settings of *special_bonds* command can remove pairwise interactions between atoms in the same bond, angle, or dihedral. This is the default setting for the *special_bonds* command, and means those pairwise interactions do not appear in the neighbor list. Because this fix uses the neighbor list, it also means those pairs will not be included in the calculation. One way to get around this, is to write a dump file, and use the *rerun* command to compute the bispectrum components for snapshots in the dump file. The rerun script can use a *special_bonds* command that includes all pairs in the neighbor list.

Output info:

Compute *sna/atom* calculates a per-atom array, each column corresponding to a particular bispectrum component. The total number of columns and the identity of the bispectrum component contained in each column depend of the value of *twojmax*, as described by the following piece of python code:

```
for j1 in range(0,twojmax+1):
    for j2 in range(0,j1+1):
        for j in range(j1-j2,min(twojmax,j1+j2)+1,2):
            if (j>=j1): print j1/2.,j2/2.,j/2.
```

Note: the *diagonal* keyword allowing other possible choices for the number of bispectrum components was removed in 2019, since all potentials use the value of 3, corresponding to the above set of bispectrum components.

Compute *snad/atom* evaluates a per-atom array. The columns are arranged into *ntypes* blocks, listed in order of atom type *I*. Each block contains three sub-blocks corresponding to the *x*, *y*, and *z* components of the atom position. Each of these sub-blocks contains one column for each bispectrum component, the same as for compute *sna/atom*

Compute *snav/atom* evaluates a per-atom array. The columns are arranged into *ntypes* blocks, listed in order of atom type *I*. Each block contains six sub-blocks corresponding to the *xx*, *yy*, *zz*, *yz*, *xz*, and *xy* components of the virial tensor in Voigt notation. Each of these sub-blocks contains one column for each bispectrum component, the same as for compute *sna/atom*

Compute *snap* evaluates a global array. The columns are arranged into *ntypes* blocks, listed in order of atom type *I*. Each block contains one column for each bispectrum component, the same as for compute *sna/atom*. A final column contains the corresponding energy, force component on an atom, or virial stress component. The rows of the array appear in the following order:

- 1 row: *sna/atom* quantities summed for all atoms of type *I*
- 3**N* rows: *snad/atom* quantities, with derivatives w.r.t. x, y, and z coordinate of atom *i* appearing in consecutive rows. The atoms are sorted based on atom ID.
- 6 rows: *snav/atom* quantities summed for all atoms of type *I*

For example, if *K* =30 and ntypes=1, the number of columns in the per-atom arrays generated by *sna/atom*, *snad/atom*, and *snav/atom* are 30, 90, and 180, respectively. With *quadratic* value=1, the numbers of columns are 930, 2790, and 5580, respectively. The number of columns in the global array generated by *snap* are 31, and 931, respectively, while the number of rows is 1+3**N*+6, where *N* is the total number of atoms.

If the *quadratic* keyword value is set to 1, then additional columns are generated, corresponding to the products of all distinct pairs of bispectrum components. If the number of bispectrum components is *K*, then the number of distinct pairs is *K*(*K*+1)/2. For compute *sna/atom* these columns are appended to existing *K* columns. The ordering of quadratic terms is upper-triangular, (1,1),(1,2)…(1,*K*),(2,1)…(*K*-1,*K*-1),(*K*-1,*K*),(*K*,*K*). For computes *snad/atom* and *snav/atom* each set of *K*(*K*+1)/2 additional columns is inserted directly after each of sub-block of linear terms i.e. linear and quadratic terms are contiguous. So the nesting order from inside to outside is bispectrum component, linear then quadratic, vector/tensor component, type.

These values can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

17.106.4 Restrictions

These computes are part of the SNAP package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.106.5 Related commands

pair_style snap

17.106.6 Default

The optional keyword defaults are *rmin0* = 0, *switchflag* = 1, *bzeroflag* = 1, *quadraticflag* = 0,

---

(Thompson) Thompson, Swiler, Trott, Foiles, Tucker, under review, preprint available at arXiv:1409.3880

(Bartok) Bartok, Payne, Risi, Csanyi, Phys Rev Lett, 104, 136403 (2010).

(Meremianin) Meremianin, J. Phys. A, 39, 3099 (2006).

(Varshalovich) Varshalovich, Moskalev, Khersonskii, Quantum Theory of Angular Momentum, World Scientific, Singapore (1987).

17.107 compute spin command

17.107.1 Syntax

```
compute ID group-ID spin
```

- ID, group-ID are documented in *compute* command
- spin = style name of this compute command

17.107.2 Examples

```
compute out_mag all spin
```

17.107.3 Description

Define a computation that calculates magnetic quantities for a system of atoms having spins.

This compute calculates the following 6 magnetic quantities:

- the three first quantities are the x,y and z coordinates of the total magnetization,
- the fourth quantity is the norm of the total magnetization,
- The fifth quantity is the magnetic energy (in eV),
- The sixth one is referred to as the spin temperature, according to the work of *(Nurdin)*.

The simplest way to output the results of the compute spin calculation is to define some of the quantities as variables, and to use the thermo and thermo_style commands, for example:

```
compute out_mag         all spin

variable mag_z          equal c_out_mag[3]
variable mag_norm       equal c_out_mag[4]
variable temp_mag       equal c_out_mag[6]

thermo                  10
thermo_style            custom step v_mag_z v_mag_norm v_temp_mag
```

This series of commands evaluates the total magnetization along z, the norm of the total magnetization, and the magnetic temperature. Three variables are assigned to those quantities. The thermo and thermo_style commands print them every 10 timesteps.

Output info:

The array values are "intensive". The array values will be in metal units (*units*).

17.107.4 Restrictions

The *spin* compute is part of the SPIN package. This compute is only enabled if LAMMPS was built with this package. See the *Build package* doc page for more info. The atom_style has to be "spin" for this compute to be valid.

Related commands:

none

Default:

none

(Nurdin) Nurdin and Schotte Phys Rev E, 61(4), 3579 (2000)

17.108 compute stress/atom command

17.109 compute centroid/stress/atom command

17.109.1 Syntax

```
compute ID group-ID style temp-ID keyword ...
```

- ID, group-ID are documented in *compute* command
- style = *stress/atom* or *centroid/stress/atom*
- temp-ID = ID of compute that calculates temperature, can be NULL if not needed
- zero or more keywords may be appended
- keyword = *ke* or *pair* or *bond* or *angle* or *dihedral* or *improper* or *kspace* or *fix* or *virial*

17.109.2 Examples

```
compute 1 mobile stress/atom NULL
compute 1 mobile stress/atom myRamp
compute 1 all stress/atom NULL pair bond
compute 1 all centroid/stress/atom NULL bond dihedral improper
```

17.109.3 Description

Define a computation that computes per-atom stress tensor for each atom in a group. In case of compute *stress/atom*, the tensor for each atom is symmetric with 6 components and is stored as a 6-element vector in the following order: xx, yy, zz, xy, xz, yz. In case of compute *centroid/stress/atom*, the tensor for each atom is asymmetric with 9 components and is stored as a 9-element vector in the following order: xx, yy, zz, xy, xz, yz, yx, zx, zy. See the *compute pressure* command if you want the stress tensor (pressure) of the entire system.

The stress tensor for atom I is given by the following formula, where a and b take on values x, y, z to generate the components of the tensor:

$$S_{ab} = -mv_a v_b - W_{ab}$$

The first term is a kinetic energy contribution for atom I. See details below on how the specified *temp-ID* can affect the velocities used in this calculation. The second term is the virial contribution due to intra and intermolecular interactions, where the exact computation details are determined by the compute style.

In case of compute *stress/atom*, the virial contribution is:

$$\begin{aligned} W_{ab} = & \frac{1}{2}\sum_{n=1}^{N_p}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b}) + \frac{1}{2}\sum_{n=1}^{N_b}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b}) \\ & + \frac{1}{3}\sum_{n=1}^{N_a}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b} + r_{3_a}F_{3_b}) + \frac{1}{4}\sum_{n=1}^{N_d}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b} + r_{3_a}F_{3_b} + r_{4_a}F_{4_b}) \\ & + \frac{1}{4}\sum_{n=1}^{N_i}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b} + r_{3_a}F_{3_b} + r_{4_a}F_{4_b}) + \mathrm{Kspace}(r_{i_a}, F_{i_b}) + \sum_{n=1}^{N_f} r_{i_a}F_{i_b} \end{aligned}$$

The first term is a pairwise energy contribution where n loops over the N_p neighbors of atom I, $\mathbf{r}_1$ and $\mathbf{r}_2$ are the positions of the 2 atoms in the pairwise interaction, and $\mathbf{F}_1$ and $\mathbf{F}_2$ are the forces on the 2 atoms resulting from the pairwise interaction. The second term is a bond contribution of similar form for the N_b bonds which atom I is part of. There are similar terms for the N_a angle, N_d dihedral, and N_i improper interactions atom I is part of. There is also a term for the KSpace contribution from long-range Coulombic interactions, if defined. Finally, there is a term for the N_f *fixes* that apply internal constraint forces to atom I. Currently, only the *fix shake* and *fix rigid* commands contribute to this term. As the coefficients in the formula imply, a virial contribution produced by a small set of atoms (e.g. 4 atoms in a dihedral or 3 atoms in a Tersoff 3-body interaction) is assigned in equal portions to each atom in the set. E.g. 1/4 of the dihedral virial to each of the 4 atoms, or 1/3 of the fix virial due to SHAKE constraints applied to atoms in a water molecule via the *fix shake* command.

In case of compute *centroid/stress/atom*, the virial contribution is:

$$\begin{aligned} W_{ab} = & \sum_{n=1}^{N_p} r_{I0_a}F_{I_b} + \sum_{n=1}^{N_b} r_{I0_a}F_{I_b} + \sum_{n=1}^{N_a} r_{I0_a}F_{I_b} + \sum_{n=1}^{N_d} r_{I0_a}F_{I_b} + \sum_{n=1}^{N_i} r_{I0_a}F_{I_b} \\ & + \mathrm{Kspace}(r_{i_a}, F_{i_b}) + \sum_{n=1}^{N_f} r_{i_a}F_{i_b} \end{aligned}$$

As with compute *stress/atom*, the first, second, third, fourth and fifth terms are pairwise, bond, angle, dihedral and improper contributions, but instead of assigning the virial contribution equally to each atom, only the force $\mathbf{F}_I$ acting on atom I due to the interaction and the relative position $\mathbf{r}_{I0}$ of the atom I to the geometric center of the interacting atoms, i.e. centroid, is used. As the geometric center is different for each interaction, the $\mathbf{r}_{I0}$ also differs. The sixth and seventh terms, Kspace and *fix* contribution respectively, are computed identical to compute *stress/atom*. Although the total system virial is the same as compute *stress/atom*, compute *centroid/stress/atom* is know to result in more consistent heat flux values for angle, dihedrals and improper contributions when computed via *compute heat/flux*.

If no extra keywords are listed, the kinetic contribution all of the virial contribution terms are included in the per-atom stress tensor. If any extra keywords are listed, only those terms are summed to compute the tensor. The *virial* keyword means include all terms except the kinetic energy *ke*.

Note that the stress for each atom is due to its interaction with all other atoms in the simulation, not just with other atoms in the group.

Details of how compute *stress/atom* obtains the virial for individual atoms for either pairwise or many-body potentials, and including the effects of periodic boundary conditions is discussed in *(Thompson)*. The basic idea for many-body potentials is to treat each component of the force computation between a small cluster of atoms in the same manner as in the formula above for bond, angle, dihedral, etc interactions. Namely the quantity $\mathbf{r} \cdot \mathbf{F}$ is summed over the atoms in the interaction, with the r vectors unwrapped by periodic boundaries so that the cluster of atoms is close together. The total contribution for the cluster interaction is divided evenly among those atoms. Details of how compute *centroid/stress/atom* obtains the virial for individual atoms is given in *(Surblys)*, where the idea is that the virial of the atom I is the result of only the force $\mathbf{F}_I$ on the atom due to the interaction and its positional vector $\mathbf{r}_{I0}$, relative to the geometric center of the interacting atoms, regardless of the number of participating atoms. The periodic boundary treatment is identical to that of compute *stress/atom*, and both of them reduce to identical expressions for two-body interactions, i.e. computed values for contributions from bonds and two-body pair styles, such as *Lennard-Jones*, will be the same, while contributions from angles, dihedrals and impropers will be different.

The *dihedral_style charmm* style calculates pairwise interactions between 1-4 atoms. The virial contribution of these terms is included in the pair virial, not the dihedral virial.

The KSpace contribution is calculated using the method in *(Heyes)* for the Ewald method and by the methodology described in *(Sirk)* for PPPM. The choice of KSpace solver is specified by the *kspace_style pppm* command. Note that for PPPM, the calculation requires 6 extra FFTs each timestep that per-atom stress is calculated. Thus it can significantly increase the cost of the PPPM calculation if it is needed on a large fraction of the simulation timesteps.

The *temp-ID* argument can be used to affect the per-atom velocities used in the kinetic energy contribution to the total stress. If the kinetic energy is not included in the stress, than the temperature compute is not used and can be specified as NULL. If the kinetic energy is included and you wish to use atom velocities as-is, then *temp-ID* can also be specified as NULL. If desired, the specified temperature compute can be one that subtracts off a bias to leave each atom with only a thermal velocity to use in the formula above, e.g. by subtracting a background streaming velocity. See the doc pages for individual *compute commands* to determine which ones include a bias.

Note that as defined in the formula, per-atom stress is the negative of the per-atom pressure tensor. It is also really a stress*volume formulation, meaning the computed quantity is in units of pressure*volume. It would need to be divided by a per-atom volume to have units of stress (pressure), but an individual atom's volume is not well defined or easy to compute in a deformed solid or a liquid. See the *compute voronoi/atom* command for one possible way to estimate a per-atom volume.

Thus, if the diagonal components of the per-atom stress tensor are summed for all atoms in the system and the sum is divided by dV, where d = dimension and V is the volume of the system, the result should be $-P$, where P is the total pressure of the system.

These lines in an input script for a 3d system should yield that result. I.e. the last 2 columns of thermo output will be the same:

```
compute        peratom all stress/atom NULL
compute        p all reduce sum c_peratom[1] c_peratom[2] c_peratom[3]
variable       press equal -(c_p[1]+c_p[2]+c_p[3])/(3*vol)
thermo_style   custom step temp etotal press v_press
```

Note: The per-atom stress does not include any Lennard-Jones tail corrections to the pressure added by the *pair_modify tail yes* command, since those are contributions to the global system pressure.

Output info:

This compute *stress/atom* calculates a per-atom array with 6 columns, which can be accessed by indices 1-6 by any command that uses per-atom values from a compute as input. The compute *centroid/stress/atom* produces a per-atom

array with 9 columns, but otherwise can be used in an identical manner to compute *stress/atom*. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom array values will be in pressure*volume *units* as discussed above.

17.109.4 Restrictions

Currently, compute *centroid/stress/atom* does not support pair styles with many-body interactions, such as *Tersoff*, and LAMMPS will generate an error in such cases. In principal, equivalent formulation to that of angle, dihedral and improper contributions in the virial W_{ab} formula can also be applied to the many-body pair styles, and is planned in the future.

17.109.5 Related commands

compute pe, *compute pressure*

Default: none

(Heyes) Heyes, Phys Rev B, 49, 755 (1994).

(Sirk) Sirk, Moore, Brown, J Chem Phys, 138, 064505 (2013).

(Thompson) Thompson, Plimpton, Mattson, J Chem Phys, 131, 154107 (2009).

(Surblys) Surblys, Matsubara, Kikugawa, Ohara, Phys Rev E, 99, 051301(R) (2019).

17.110 compute stress/mop command

17.111 compute stress/mop/profile command

17.111.1 Syntax

```
compute ID group-ID style dir args keywords ...
```

- ID, group-ID are documented in *compute* command
- style = *stress/mop* or *stress/mop/profile*
- dir = *x* or *y* or *z* is the direction normal to the plane
- args = argument specific to the compute style
- keywords = *kin* or *conf* or *total* (one of more can be specified)

```
  stress/mop args = pos
    pos = lower or center or upper or coordinate value (distance units) is␣
↪the position of the plane
  stress/mop/profile args = origin delta
    origin = lower or center or upper or coordinate value (distance units) is␣
↪the position of the first plane
    delta = value (distance units) is the distance between planes

compute 1 all stress/mop x lower total
```

```
compute 1 liquid stress/mop z 0.0 kin conf
fix 1 all ave/time 10 1000 10000 c_1[*] file mop.time
fix 1 all ave/time 10 1000 10000 c_1[2] file mop.time

compute 1 all stress/mop/profile x lower 0.1 total
compute 1 liquid stress/mop/profile z 0.0 0.25 kin conf
fix 1 all ave/time 500 20 10000 c_1[*] ave running overwrite file mopp.time␣
↪mode vector
```

17.111.2 Description

Compute *stress/mop* and compute *stress/mop/profile* define computations that calculate components of the local stress tensor using the method of planes *(Todd)*. Specifically in compute *stress/mop* calculates 3 components are computed in directions *dir*,*x*; *dir*,*y*; and *dir*,*z*; where *dir* is the direction normal to the plane, while in compute *stress/mop/profile* the profile of the stress is computed.

Contrary to methods based on histograms of atomic stress (i.e. using *compute stress/atom*), the method of planes is compatible with mechanical balance in heterogeneous systems and at interfaces *(Todd)*.

The stress tensor is the sum of a kinetic term and a configurational term, which are given respectively by Eq. (21) and Eq. (16) in *(Todd)*. For the kinetic part, the algorithm considers that atoms have crossed the plane if their positions at times t-dt and t are one on either side of the plane, and uses the velocity at time t-dt/2 given by the velocity-Verlet algorithm.

Between one and three keywords can be used to indicate which contributions to the stress must be computed: kinetic stress (kin), configurational stress (conf), and/or total stress (total).

NOTE 1: The configurational stress is computed considering all pairs of atoms where at least one atom belongs to group group-ID.

NOTE 2: The local stress does not include any Lennard-Jones tail corrections to the pressure added by the *pair_modify tail yes* command, since those are contributions to the global system pressure.

Output info:

Compute *stress/mop* calculates a global vector (indices starting at 1), with 3 values for each declared keyword (in the order the keywords have been declared). For each keyword, the stress tensor components are ordered as follows: stress_dir,x, stress_dir,y, and stress_dir,z.

Compute *stress/mop/profile* instead calculates a global array, with 1 column giving the position of the planes where the stress tensor was computed, and with 3 columns of values for each declared keyword (in the order the keywords have been declared). For each keyword, the profiles of stress tensor components are ordered as follows: stress_dir,x; stress_dir,y; and stress_dir,z.

The values are in pressure *units*.

The values produced by this compute can be accessed by various *output commands*. For instance, the results can be written to a file using the *fix ave/time* command. Please see the example in the examples/USER/mop folder.

17.111.3 Restrictions

These styles are part of the USER-MISC package. They are only enabled if LAMMPS is built with that package. See the *Build package* doc page on for more info.

The method is only implemented for 3d orthogonal simulation boxes whose size does not change in time, and axis-aligned planes.

The method only works with two-body pair interactions, because it requires the class method pair->single() to be implemented. In particular, it does not work with more than two-body pair interactions, intra-molecular interactions, and long range (kspace) interactions.

17.111.4 Related commands

compute stress/atom

Default: none

(Todd) B. D. Todd, Denis J. Evans, and Peter J. Daivis: "Pressure tensor for inhomogeneous fluids", Phys. Rev. E 52, 1627 (1995).

17.112 compute force/tally command

17.113 compute heat/flux/tally command

17.114 compute pe/tally command

17.115 compute pe/mol/tally command

17.116 compute stress/tally command

17.116.1 Syntax

```
compute ID group-ID style group2-ID
```

- ID, group-ID are documented in *compute* command
- style = *force/tally* or *pe/tally* or *pe/mol/tally* or *stress/tally*
- group2-ID = group ID of second (or same) group

17.116.2 Examples

```
compute 1 lower force/tally upper
compute 1 left pe/tally right
compute 1 lower stress/tally lower
```

17.116.3 Description

Define a computation that calculates properties between two groups of atoms by accumulating them from pairwise non-bonded computations. The two groups can be the same. This is similar to *compute group/group* only that the data is accumulated directly during the non-bonded force computation. The computes *force/tally*, *pe/tally*, *stress/tally*, and *heat/flux/tally* are primarily provided as example how to program additional, more sophisticated computes using the tally callback mechanism. Compute *pe/mol/tally* is one such style, that can - through using this mechanism - separately tally intermolecular and intramolecular energies. Something that would otherwise be impossible without integrating this as a core functionality into the based classes of LAMMPS.

The pairwise contributions are computing via a callback that the compute registers with the non-bonded pairwise force computation. This limits the use to systems that have no bonds, no Kspace, and no many-body interactions. On the other hand, the computation does not have to compute forces or energies a second time and thus can be much more efficient. The callback mechanism allows to write more complex pairwise property computations.

Output info:

Compute *pe/tally* calculates a global scalar (the energy) and a per atom scalar (the contributions of the single atom to the global scalar). Compute *pe/mol/tally* calculates a global 4-element vector containing (in this order): *evdwl* and *ecoul* for intramolecular pairs and *evdwl* and *ecoul* for intermolecular pairs. Since molecules are identified by their molecule IDs, the partitioning does not have to be related to molecules, but the energies are tallied into the respective slots depending on whether the molecule IDs of a pair are the same or different. Compute *force/tally* calculates a global scalar (the force magnitude) and a per atom 3-element vector (force contribution from each atom). Compute *stress/tally* calculates a global scalar (average of the diagonal elements of the stress tensor) and a per atom vector (the 6 elements of stress tensor contributions from the individual atom).

Both the scalar and vector values calculated by this compute are "extensive".

17.116.4 Restrictions

This compute is part of the USER-TALLY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Not all pair styles can be evaluated in a pairwise mode as required by this compute. For example, 3-body and other many-body potentials, such as *Tersoff* and *Stillinger-Weber* cannot be used. *EAM* potentials only include the pair potential portion of the EAM interaction when used by this compute, not the embedding term. Also bonded or Kspace interactions do not contribute to this compute.

The computes in this package are not compatible with dynamic groups.

17.116.5 Related commands

*compute group/group*_compute_group_group.html, *compute heat/flux*_compute_heat_flux.html

Default: none

17.117 compute tdpd/cc/atom command

17.117.1 Syntax

```
compute ID group-ID tdpd/cc/atom index
```

- ID, group-ID are documented in *compute* command
- tdpd/cc/atom = style name of this compute command
- index = index of chemical species (1 to Nspecies)

17.117.2 Examples

```
compute 1 all tdpd/cc/atom 2
```

17.117.3 Description

Define a computation that calculates the per-atom chemical concentration of a specified species for each tDPD particle in a group.

The chemical concentration of each species is defined as the number of molecules carried by a tDPD particle for dilute solution. For more details see *(Li2015)*.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The per-atom vector values will be in the units of chemical species per unit mass.

17.117.4 Restrictions

This compute is part of the USER-MESO package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.117.5 Related commands

pair_style tdpd

Default: none

(Li2015) Li, Yazdani, Tartakovsky, Karniadakis, J Chem Phys, 143: 014101 (2015). DOI: 10.1063/1.4923254

17.118 compute temp command

17.119 compute temp/kk command

17.119.1 Syntax

```
compute ID group-ID temp
```

- ID, group-ID are documented in *compute* command
- temp = style name of this compute command

17.119.2 Examples

```
compute 1 all temp
compute myTemp mobile temp
```

17.119.3 Description

Define a computation that calculates the temperature of a group of atoms. A compute of this style can be used by any command that computes a temperature, e.g. *thermo_modify*, *fix temp/rescale*, *fix npt*, etc.

The temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the *compute_modify* command if this is not the case.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as *fix shake* and *fix rigid*. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the *compute_modify* command.

A compute of this style with the ID of "thermo_temp" is created when LAMMPS starts up, as if this command were in the input script:

```
compute thermo_temp all temp
```

See the "thermo_style" command for more details.

See the *Howto thermostat* doc page for a discussion of different ways to compute temperature and perform thermostatting.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature *units*. The vector values will be in energy *units*.

17.119.4 Restrictions

none

17.119.5 Related commands

compute temp/partial, *compute temp/region*, *compute pressure*

Default: none

17.120 compute temp/asphere command

17.120.1 Syntax

```
compute ID group-ID temp/asphere keyword value ...
```

- ID, group-ID are documented in *compute* command
- temp/asphere = style name of this compute command
- zero or more keyword/value pairs may be appended
- keyword = *bias* or *dof*

```
bias value = bias-ID
  bias-ID = ID of a temperature compute that removes a velocity bias
dof value = all or rotate
  all = compute temperature of translational and rotational degrees of␣
↪freedom
  rotate = compute temperature of just rotational degrees of freedom
```

17.120.2 Examples

```
compute 1 all temp/asphere
compute myTemp mobile temp/asphere bias tempCOM
compute myTemp mobile temp/asphere dof rotate
```

17.120.3 Description

Define a computation that calculates the temperature of a group of aspherical particles, including a contribution from both their translational and rotational kinetic energy. This differs from the usual *compute temp* command, which assumes point particles with only translational kinetic energy.

Only finite-size particles (aspherical or spherical) can be included in the group. For 3d finite-size particles, each has 6 degrees of freedom (3 translational, 3 rotational). For 2d finite-size particles, each has 3 degrees of freedom (2 translational, 1 rotational).

Note: This choice for degrees of freedom (dof) assumes that all finite-size aspherical or spherical particles in your model will freely rotate, sampling all their rotational dof. It is possible to use a combination of interaction potentials and fixes that induce no torque or otherwise constrain some of all of your particles so that this is not the case. Then there are less dof and you should use the *compute_modify extra* command to adjust the dof accordingly.

For example, an aspherical particle with all three of its shape parameters the same is a sphere. If it does not rotate, then it should have 3 dof instead of 6 in 3d (or 2 instead of 3 in 2d). A uniaxial aspherical particle has two of its three shape parameters the same. If it does not rotate around the axis perpendicular to its circular cross section, then it should have 5 dof instead of 6 in 3d. The latter is the case for uniaxial ellipsoids in a *GayBerne model* since there is no induced torque around the optical axis. It will also be the case for bi-axial ellipsoids when exactly two of the semiaxes have the same length and the corresponding relative well depths are equal.

The translational kinetic energy is computed the same as is described by the *compute temp* command. The rotational kinetic energy is computed as 1/2 I w^2, where I is the inertia tensor for the aspherical particle and w is its angular velocity, which is computed from its angular momentum.

Note: For *2d models*, particles are treated as ellipsoids, not ellipses, meaning their moments of inertia will be the same as in 3d.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute. The formula for the components of the tensor is the same as the above formula, except that v^2 and w^2 are replaced by vx*vy and wx*wy for the xy component, and the appropriate elements of the inertia tensor are used. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the *compute_modify* command if this is not the case.

This compute subtracts out translational degrees-of-freedom due to fixes that constrain molecular motion, such as *fix shake* and *fix rigid*. This means the temperature of groups of atoms that include these constraints will be computed

correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the *compute_modify* command.

See the *Howto thermostat* doc page for a discussion of different ways to compute temperature and perform thermostatting.

The keyword/value option pairs are used in the following ways.

For the *bias* keyword, *bias-ID* refers to the ID of a temperature compute that removes a "bias" velocity from each atom. This allows compute temp/sphere to compute its thermal temperature after the translational kinetic energy components have been altered in a prescribed way, e.g. to remove a flow velocity profile. Thermostats that use this compute will work with this bias term. See the doc pages for individual computes that calculate a temperature and the doc pages for fixes that perform thermostatting for more details.

For the *dof* keyword, a setting of *all* calculates a temperature that includes both translational and rotational degrees of freedom. A setting of *rotate* calculates a temperature that includes only rotational degrees of freedom.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature *units*. The vector values will be in energy *units*.

17.120.4 Restrictions

This compute is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This compute requires that atoms store angular momentum and a quaternion as defined by the *atom_style ellipsoid* command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or spherical as defined by their shape attribute.

17.120.5 Related commands

compute temp

Default: none

17.121 compute temp/body command

17.121.1 Syntax

```
compute ID group-ID temp/body keyword value ...
```

- ID, group-ID are documented in *compute* command
- temp/body = style name of this compute command

- zero or more keyword/value pairs may be appended
- keyword = *bias* or *dof*

```
bias value = bias-ID
  bias-ID = ID of a temperature compute that removes a velocity bias
dof value = all or rotate
  all = compute temperature of translational and rotational degrees of␣
↪freedom
  rotate = compute temperature of just rotational degrees of freedom
```

17.121.2 Examples

```
compute 1 all temp/body
compute myTemp mobile temp/body bias tempCOM
compute myTemp mobile temp/body dof rotate
```

17.121.3 Description

Define a computation that calculates the temperature of a group of body particles, including a contribution from both their translational and rotational kinetic energy. This differs from the usual *compute temp* command, which assumes point particles with only translational kinetic energy.

Only body particles can be included in the group. For 3d particles, each has 6 degrees of freedom (3 translational, 3 rotational). For 2d body particles, each has 3 degrees of freedom (2 translational, 1 rotational).

Note: This choice for degrees of freedom (dof) assumes that all body particles in your model will freely rotate, sampling all their rotational dof. It is possible to use a combination of interaction potentials and fixes that induce no torque or otherwise constrain some of all of your particles so that this is not the case. Then there are less dof and you should use the *compute_modify extra* command to adjust the dof accordingly.

The translational kinetic energy is computed the same as is described by the *compute temp* command. The rotational kinetic energy is computed as 1/2 I w^2, where I is the inertia tensor for the aspherical particle and w is its angular velocity, which is computed from its angular momentum.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute. The formula for the components of the tensor is the same as the above formula, except that v^2 and w^2 are replaced by vx*vy and wx*wy for the xy component, and the appropriate elements of the inertia tensor are used. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the *compute_modify* command if this is not the case.

This compute subtracts out translational degrees-of-freedom due to fixes that constrain molecular motion, such as *fix shake* and *fix rigid*. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the *compute_modify* command.

See the *Howto thermostat* doc page for a discussion of different ways to compute temperature and perform thermostatting.

The keyword/value option pairs are used in the following ways.

For the *bias* keyword, *bias-ID* refers to the ID of a temperature compute that removes a "bias" velocity from each atom. This allows compute temp/sphere to compute its thermal temperature after the translational kinetic energy components have been altered in a prescribed way, e.g. to remove a flow velocity profile. Thermostats that use this compute will work with this bias term. See the doc pages for individual computes that calculate a temperature and the doc pages for fixes that perform thermostatting for more details.

For the *dof* keyword, a setting of *all* calculates a temperature that includes both translational and rotational degrees of freedom. A setting of *rotate* calculates a temperature that includes only rotational degrees of freedom.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature *units*. The vector values will be in energy *units*.

17.121.4 Restrictions

This compute is part of the BODY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This compute requires that atoms store angular momentum and a quaternion as defined by the *atom_style body* command.

17.121.5 Related commands

compute temp

Default: none

17.122 compute temp/chunk command

17.122.1 Syntax

```
compute ID group-ID temp/chunk chunkID value1 value2 ... keyword value ...
```

- ID, group-ID are documented in *compute* command
- temp/chunk = style name of this compute command
- chunkID = ID of *compute chunk/atom* command
- zero or more values can be listed as value1,value2,etc
- value = *temp* or *kecom* or *internal*

```
temp = temperature of each chunk
kecom = kinetic energy of each chunk based on velocity of center of mass
internal = internal kinetic energy of each chunk
```

- zero or more keyword/value pairs may be appended

- keyword = *com* or *bias* or *adof* or *cdof*

```
com value = yes or no
  yes = subtract center-of-mass velocity from each chunk before␣
↪calculating temperature
  no = do not subtract center-of-mass velocity
bias value = bias-ID
  bias-ID = ID of a temperature compute that removes a velocity bias
adof value = dof_per_atom
  dof_per_atom = define this many degrees-of-freedom per atom
cdof value = dof_per_chunk
  dof_per_chunk = define this many degrees-of-freedom per chunk
```

17.122.2 Examples

```
compute 1 fluid temp/chunk molchunk
compute 1 fluid temp/chunk molchunk temp internal
compute 1 fluid temp/chunk molchunk bias tpartial adof 2.0
```

17.122.3 Description

Define a computation that calculates the temperature of a group of atoms that are also in chunks, after optionally subtracting out the center-of-mass velocity of each chunk. By specifying optional values, it can also calculate the per-chunk temperature or energies of the multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a *compute chunk/atom* command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the *compute chunk/atom* and *Howto chunk* doc pages for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

The temperature is calculated by the formula KE = DOF/2 k T, where KE = total kinetic energy of all atoms assigned to chunks (sum of 1/2 m v^2), DOF = the total number of degrees of freedom for those atoms, k = Boltzmann constant, and T = temperature.

The DOF is calculated as N*adof + Nchunk*cdof, where N = number of atoms contributing to the KE, adof = degrees of freedom per atom, and cdof = degrees of freedom per chunk. By default adof = 2 or 3 = dimensionality of system, as set via the *dimension* command, and cdof = 0.0. This gives the usual formula for temperature.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

Note that the number of atoms contributing to the temperature is calculated each time the temperature is evaluated since it is assumed the atoms may be dynamically assigned to chunks. Thus there is no need to use the *dynamic* option of the *compute_modify* command for this compute style.

If any optional values are specified, then per-chunk quantities are also calculated and stored in a global array, as described below.

The *temp* value calculates the temperature for each chunk by the formula KE = DOF/2 k T, where KE = total kinetic energy of the chunk of atoms (sum of 1/2 m v^2), DOF = the total number of degrees of freedom for all atoms in the chunk, k = Boltzmann constant, and T = temperature.

The DOF in this case is calculated as N*adof + cdof, where N = number of atoms in the chunk, adof = degrees of freedom per atom, and cdof = degrees of freedom per chunk. By default adof = 2 or 3 = dimensionality of system, as set via the *dimension* command, and cdof = 0.0. This gives the usual formula for temperature.

The *kecom* value calculates the kinetic energy of each chunk as if all its atoms were moving with the velocity of the center-of-mass of the chunk.

The *internal* value calculates the internal kinetic energy of each chunk. The interal KE is summed over the atoms in the chunk using an internal "thermal" velocity for each atom, which is its velocity minus the center-of-mass velocity of the chunk.

Note that currently the global and per-chunk temperatures calculated by this compute only include translational degrees of freedom for each atom. No rotational degrees of freedom are included for finite-size particles. Also no degrees of freedom are subtracted for any velocity bias or constraints that are applied, such as *compute temp/partial*, or *fix shake* or *fix rigid*. This is because those degrees of freedom (e.g. a constrained bond) could apply to sets of atoms that are both included and excluded from a specific chunk, and hence the concept is somewhat ill-defined. In some cases, you can use the *adof* and *cdof* keywords to adjust the calculated degrees of freedom appropriately, as explained below.

Note that the per-chunk temperature calculated by this compute and the *fix ave/chunk temp* command can be different. This compute calculates the temperature for each chunk for a single snapshot. Fix ave/chunk can do that but can also time average those values over many snapshots, or it can compute a temperature as if the atoms in the chunk on different timesteps were collected together as one set of atoms to calculate their temperature. This compute allows the center-of-mass velocity of each chunk to be subtracted before calculating the temperature; fix ave/chunk does not.

Note: Only atoms in the specified group contribute to the calculations performed by this compute. The *compute chunk/atom* command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

The simplest way to output the per-chunk results of the compute temp/chunk calculation to a file is to use the *fix ave/time* command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all temp/chunk cc1 temp
fix 1 all ave/time 100 1 100 c_myChunk file tmp.out mode vector
```

The keyword/value option pairs are used in the following ways.

The *com* keyword can be used with a value of *yes* to subtract the velocity of the center-of-mass for each chunk from the velocity of the atoms in that chunk, before calculating either the global or per-chunk temperature. This can be useful if the atoms are streaming or otherwise moving collectively, and you wish to calculate only the thermal temperature.

For the *bias* keyword, *bias-ID* refers to the ID of a temperature compute that removes a "bias" velocity from each atom. This also allows calculation of the global or per-chunk temperature using only the thermal temperature of atoms in each chunk after the translational kinetic energy components have been altered in a prescribed way, e.g. to remove a velocity profile. It also applies to the calculation of the other per-chunk values, such as *kecom* or *internal*, which involve the center-of-mass velocity of each chunk, which is calculated after the velocity bias is removed from each atom. Note that the temperature compute will apply its bias globally to the entire system, not on a per-chunk basis.

The *adof* and *cdof* keywords define the values used in the degree of freedom (DOF) formulas used for the global or per-chunk temperature, as described above. They can be used to calculate a more appropriate temperature for some kinds of chunks. Here are 3 examples:

If spatially binned chunks contain some number of water molecules and *fix shake* is used to make each molecule rigid, then you could calculate a temperature with 6 degrees of freedom (DOF) (3 translational, 3 rotational) per molecule by setting *adof* to 2.0.

If *compute temp/partial* is used with the *bias* keyword to only allow the x component of velocity to contribute to the temperature, then *adof* = 1.0 would be appropriate.

If each chunk consists of a large molecule, with some number of its bonds constrained by *fix shake* or the entire molecule by *fix rigid/small*, *adof* = 0.0 and *cdof* could be set to the remaining degrees of freedom for the entire molecule (entire chunk in this case), e.g. 6 for 3d, or 3 for 2d, for a rigid molecule.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

This compute also optionally calculates a global array, if one or more of the optional values are specified. The number of rows in the array = the number of chunks *Nchunk* as calculated by the specified *compute chunk/atom* command. The number of columns is the number of specified values (1 or more). These values can be accessed by any command that uses global array values from a compute as input. Again, see the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive". The array values are "intensive".

The scalar value will be in temperature *units*. The vector values will be in energy *units*. The array values will be in temperature *units* for the *temp* value, and in energy *units* for the *kecom* and *internal* values.

17.122.4 Restrictions

The *com* and *bias* keywords cannot be used together.

17.122.5 Related commands

compute temp, *fix ave/chunk temp*

17.122.6 Default

The option defaults are com no, no bias, adof = dimensionality of the system (2 or 3), and cdof = 0.0.

17.123 compute temp/com command

17.123.1 Syntax

```
compute ID group-ID temp/com
```

- ID, group-ID are documented in *compute* command
- temp/com = style name of this compute command

17.123.2 Examples

```
compute 1 all temp/com
compute myTemp mobile temp/com
```

17.123.3 Description

Define a computation that calculates the temperature of a group of atoms, after subtracting out the center-of-mass velocity of the group. This is useful if the group is expected to have a non-zero net velocity for some reason. A compute of this style can be used by any command that computes a temperature, e.g. *thermo_modify*, *fix temp/rescale*, *fix npt*, etc.

After the center-of-mass velocity has been subtracted from each atom, the temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the *compute_modify* command if this is not the case.

The removal of the center-of-mass velocity by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include *fix nvt*, *fix temp/rescale*, *fix temp/berendsen*, and *fix langevin*.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as *fix shake* and *fix rigid*. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the *compute_modify* command.

See the *Howto thermostat* doc page for a discussion of different ways to compute temperature and perform thermostatting.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature *units*. The vector values will be in energy *units*.

17.123.4 Restrictions

none

17.123.5 Related commands

compute temp

Default: none

17.124 compute temp/cs command

17.124.1 Syntax

```
compute ID group-ID temp/cs group1 group2
```

- ID, group-ID are documented in *compute* command
- temp/cs = style name of this compute command
- group1 = group-ID of either cores or shells
- group2 = group-ID of either shells or cores

17.124.2 Examples

```
compute oxygen_c-s all temp/cs O_core O_shell
compute core_shells all temp/cs cores shells
```

17.124.3 Description

Define a computation that calculates the temperature of a system based on the center-of-mass velocity of atom pairs that are bonded to each other. This compute is designed to be used with the adiabatic core/shell model of *(Mitchell and Finchham)*. See the *Howto coreshell* doc page for an overview of the model as implemented in LAMMPS. Specifically, this compute enables correct temperature calculation and thermostatting of core/shell pairs where it is desirable for the internal degrees of freedom of the core/shell pairs to not be influenced by a thermostat. A compute of this style can be used by any command that computes a temperature via *fix_modify* e.g. *fix temp/rescale*, *fix npt*, etc.

Note that this compute does not require all ions to be polarized, hence defined as core/shell pairs. One can mix core/shell pairs and ions without a satellite particle if desired. The compute will consider the non-polarized ions according to the physical system.

For this compute, core and shell particles are specified by two respective group IDs, which can be defined using the *group* command. The number of atoms in the two groups must be the same and there should be one bond defined between a pair of atoms in the two groups. Non-polarized ions which might also be included in the treated system should not be included into either of these groups, they are taken into account by the *group-ID* (2nd argument) of the compute.

The temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature. Note that the velocity of each core or shell atom used in the KE calculation is the velocity of the center-of-mass (COM) of the core/shell pair the atom is part of.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz. In contrast to the temperature, the velocity of each core or shell atom is taken individually.

The change this fix makes to core/shell atom velocities is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. This "bias" is the velocity of the atom relative to the COM velocity of the core/shell pair. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining COM velocity will be performed, and the bias will be added back in. This means the thermostatting will effectively be performed on the core/shell pairs, instead of on the individual core and shell atoms. Thermostatting fixes that work in this way include *fix nvt*, *fix temp/rescale*, *fix temp/berendsen*, and *fix langevin*.

The internal energy of core/shell pairs can be calculated by the *compute temp/chunk* command, if chunks are defined as core/shell pairs. See the *Howto coreshell* doc page doc page for more discussion on how to do this.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature *units*. The vector values will be in energy *units*.

17.124.4 Restrictions

The number of core/shell pairs contributing to the temperature is assumed to be constant for the duration of the run. No fixes should be used which generate new molecules or atoms during a simulation.

17.124.5 Related commands

compute temp, *compute temp/chunk*

Default: none

(Mitchell and Finchham) Mitchell, Finchham, J Phys Condensed Matter, 5, 1031-1038 (1993).

17.125 compute temp/deform command

17.125.1 Syntax

```
compute ID group-ID temp/deform
```

- ID, group-ID are documented in *compute* command
- temp/deform = style name of this compute command

17.125.2 Examples

```
compute myTemp all temp/deform
```

17.125.3 Description

Define a computation that calculates the temperature of a group of atoms, after subtracting out a streaming velocity induced by the simulation box changing size and/or shape, for example in a non-equilibrium MD (NEMD) simulation. The size/shape change is induced by use of the *fix deform* command. A compute of this style is created by the *fix nvt/sllod* command to compute the thermal temperature of atoms for thermostatting purposes. A compute of this style can also be used by any command that computes a temperature, e.g. *thermo_modify*, *fix temp/rescale*, *fix npt*, etc.

The deformation fix changes the box size and/or shape over time, so each atom in the simulation box can be thought of as having a "streaming" velocity. For example, if the box is being sheared in x, relative to y, then atoms at the bottom of the box (low y) have a small x velocity, while atoms at the top of the box (hi y) have a large x velocity. This position-dependent streaming velocity is subtracted from each atom's actual velocity to yield a thermal velocity which is used to compute the temperature.

Note: *Fix deform* has an option for remapping either atom coordinates or velocities to the changing simulation box. When using this compute in conjunction with a deforming box, fix deform should NOT remap atom positions, but rather should let atoms respond to the changing box by adjusting their own velocities (or let *fix deform* remap the atom velocities, see it's remap option). If fix deform does remap atom positions, then they appear to move with the box but their velocity is not changed, and thus they do NOT have the streaming velocity assumed by this compute. LAMMPS will warn you if fix deform is defined and its remap setting is not consistent with this compute.

After the streaming velocity has been subtracted from each atom, the temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature. Note that v in the kinetic energy formula is the atom's thermal velocity.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the *compute_modify* command if this is not the case.

The removal of the box deformation velocity component by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include *fix nvt*, *fix temp/rescale*, *fix temp/berendsen*, and *fix langevin*.

Note: The temperature calculated by this compute is only accurate if the atoms are indeed moving with a stream velocity profile that matches the box deformation. If not, then the compute will subtract off an incorrect stream velocity, yielding a bogus thermal temperature. You should NOT assume that your atoms are streaming at the same rate the box is deforming. Rather, you should monitor their velocity profile, e.g. via the *fix ave/chunk* command. And you can compare the results of this compute to *compute temp/profile*, which actually calculates the stream profile before subtracting it. If the two computes do not give roughly the same temperature, then your atoms are not streaming consistent with the box deformation. See the *fix deform* command for more details on ways to get atoms to stream consistently with the box deformation.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as *fix shake* and *fix rigid*. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the *compute_modify* command.

See the *Howto thermostat* doc page for a discussion of different ways to compute temperature and perform thermostatting.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature *units*. The vector values will be in energy *units*.

17.125.4 Restrictions

none

17.125.5 Related commands

compute temp/ramp, *compute temp/profile*, *fix deform*, *fix nvt/sllod*

Default: none

17.126 compute temp/deform/eff command

17.126.1 Syntax

```
compute ID group-ID temp/deform/eff
```

- ID, group-ID are documented in *compute* command
- temp/deform/eff = style name of this compute command

17.126.2 Examples

```
compute myTemp all temp/deform/eff
```

17.126.3 Description

Define a computation that calculates the temperature of a group of nuclei and electrons in the *electron force field* model, after subtracting out a streaming velocity induced by the simulation box changing size and/or shape, for example in a non-equilibrium MD (NEMD) simulation. The size/shape change is induced by use of the *fix deform* command. A compute of this style is created by the *fix nvt/sllod/eff* command to compute the thermal temperature of atoms for thermostatting purposes. A compute of this style can also be used by any command that computes a temperature, e.g. *thermo_modify*, *fix npt/eff*, etc.

The calculation performed by this compute is exactly like that described by the *compute temp/deform* command, except that the formula for the temperature includes the radial electron velocity contributions, as discussed by the *compute*

temp/eff command. Note that only the translational degrees of freedom for each nuclei or electron are affected by the streaming velocity adjustment. The radial velocity component of the electrons is not affected.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature *units*. The vector values will be in energy *units*.

17.126.4 Restrictions

This compute is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.126.5 Related commands

compute temp/ramp, *fix deform*, *fix nvt/sllod/eff*

Default: none

17.127 compute temp/drude command

17.127.1 Syntax

```
compute ID group-ID temp/drude
```

- ID, group-ID are documented in *compute* command
- temp/drude = style name of this compute command

17.127.2 Examples

```
compute TDRUDE all temp/drude
```

17.127.3 Description

Define a computation that calculates the temperatures of core-Drude pairs. This compute is designed to be used with the *thermalized Drude oscillator model*. Polarizable models in LAMMPS are described on the *Howto polarizable* doc page.

Drude oscillators consist of a core particle and a Drude particle connected by a harmonic bond, and the relative motion of these Drude oscillators is usually maintained cold by a specific thermostat that acts on the relative motion of the core-Drude particle pairs. Therefore, because LAMMPS considers Drude particles as normal atoms in its default temperature compute (*compute temp* command), the reduced temperature of the core-Drude particle pairs is not calculated correctly.

By contrast, this compute calculates the temperature of the cores using center-of-mass velocities of the core-Drude pairs, and the reduced temperature of the Drude particles using the relative velocities of the Drude particles with

respect to their cores. Non-polarizable atoms are considered as cores. Their velocities contribute to the temperature of the cores.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6, which can be accessed by indices 1-6, whose components are

1. temperature of the centers of mass (temperature units)
2. temperature of the dipoles (temperature units)
3. number of degrees of freedom of the centers of mass
4. number of degrees of freedom of the dipoles
5. kinetic energy of the centers of mass (energy units)
6. kinetic energy of the dipoles (energy units)

These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

Both the scalar value and the first two values of the vector calculated by this compute are "intensive". The other 4 vector values are "extensive".

17.127.4 Restrictions

The number of degrees of freedom contributing to the temperature is assumed to be constant for the duration of the run unless the *fix_modify* command sets the option *dynamic yes*.

17.127.5 Related commands

fix drude, *fix langevin/drude*, *fix drude/transform*, *pair_style thole*, *compute temp*

Default: none

17.128 compute temp/eff command

17.128.1 Syntax

```
compute ID group-ID temp/eff
```

- ID, group-ID are documented in *compute* command
- temp/eff = style name of this compute command

17.128.2 Examples

```
compute 1 all temp/eff
compute myTemp mobile temp/eff
```

17.128.3 Description

Define a computation that calculates the temperature of a group of nuclei and electrons in the *electron force field* model. A compute of this style can be used by commands that compute a temperature, e.g. *thermo_modify*, *fix npt/eff*, etc.

The temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2 for nuclei and sum of 1/2 (m v^2 + 3/4 m s^2) for electrons, where s includes the radial electron velocity contributions), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms (only total number of nuclei in the eFF (see the *pair_eff* command) in the group, k = Boltzmann constant, and T = temperature. This expression is summed over all nuclear and electronic degrees of freedom, essentially by setting the kinetic contribution to the heat capacity to 3/2k (where only nuclei contribute). This subtlety is valid for temperatures well below the Fermi temperature, which for densities two to five times the density of liquid H2 ranges from 86,000 to 170,000 K.

Note: For eFF models, in order to override the default temperature reported by LAMMPS in the thermodynamic quantities reported via the *thermo* command, the user should apply a *thermo_modify* command, as shown in the following example:

```
compute         effTemp all temp/eff
thermo_style    custom step etotal pe ke temp press
thermo_modify   temp effTemp
```

A 6-component kinetic energy tensor is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx * vy for the xy component, etc. For the eFF, again, the radial electronic velocities are also considered.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the *compute_modify* command if this is not the case.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as *fix shake* and *fix rigid*. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the *compute_modify* command.

See the *Howto thermostat* doc page for a discussion of different ways to compute temperature and perform thermostatting.

Output info:

The scalar value calculated by this compute is "intensive", meaning it is independent of the number of atoms in the simulation. The vector values are "extensive", meaning they scale with the number of atoms in the simulation.

17.128.4 Restrictions

This compute is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.128.5 Related commands

compute temp/partial, *compute temp/region*, *compute pressure*

Default: none

17.129 compute temp/partial command

17.129.1 Syntax

```
compute ID group-ID temp/partial xflag yflag zflag
```

- ID, group-ID are documented in *compute* command
- temp/partial = style name of this compute command
- xflag,yflag,zflag = 0/1 for whether to exclude/include this dimension

17.129.2 Examples

```
compute newT flow temp/partial 1 1 0
```

17.129.3 Description

Define a computation that calculates the temperature of a group of atoms, after excluding one or more velocity components. A compute of this style can be used by any command that computes a temperature, e.g. *thermo_modify*, *fix temp/rescale*, *fix npt*, etc.

The temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature. The calculation of KE excludes the x, y, or z dimensions if xflag, yflag, or zflag = 0. The dim parameter is adjusted to give the correct number of degrees of freedom.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the calculation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the *compute_modify* command if this is not the case.

The removal of velocity components by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include *fix nvt*, *fix temp/rescale*, *fix temp/berendsen*, and *fix langevin*.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as *fix shake* and *fix rigid*. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the *compute_modify* command.

See the *Howto thermostat* doc page for a discussion of different ways to compute temperature and perform thermostatting.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature *units*. The vector values will be in energy *units*.

17.129.4 Restrictions

none

17.129.5 Related commands

compute temp, *compute temp/region*, *compute pressure*

Default: none

17.130 compute temp/profile command

17.130.1 Syntax

```
compute ID group-ID temp/profile xflag yflag zflag binstyle args
```

- ID, group-ID are documented in *compute* command
- temp/profile = style name of this compute command
- xflag,yflag,zflag = 0/1 for whether to exclude/include this dimension
- binstyle = *x* or *y* or *z* or *xy* or *yz* or *xz* or *xyz*

```
x arg = Nx
y arg = Ny
z arg = Nz
xy args = Nx Ny
yz args = Ny Nz
xz args = Nx Nz
xyz args = Nx Ny Nz
  Nx,Ny,Nz = number of velocity bins in x,y,z dimensions
```

- zero or more keyword/value pairs may be appended
- keyword = *out*

```
out value = tensor or bin
```

17.130.2 Examples

```
compute myTemp flow temp/profile 1 1 1 x 10
compute myTemp flow temp/profile 1 1 1 x 10 out bin
compute myTemp flow temp/profile 0 1 1 xyz 20 20 20
```

17.130.3 Description

Define a computation that calculates the temperature of a group of atoms, after subtracting out a spatially-averaged center-of-mass velocity field, before computing the kinetic energy. This can be useful for thermostatting a collection of atoms undergoing a complex flow, e.g. via a profile-unbiased thermostat (PUT) as described in *(Evans)*. A compute of this style can be used by any command that computes a temperature, e.g. *thermo_modify*, *fix temp/rescale*, *fix npt*, etc.

The *xflag*, *yflag*, *zflag* settings determine which components of average velocity are subtracted out.

The *binstyle* setting and its *Nx*, *Ny*, *Nz* arguments determine how bins are setup to perform spatial averaging. "Bins" can be 1d slabs, 2d pencils, or 3d bricks depending on which *binstyle* is used. The simulation box is partitioned conceptually into *Nx* by *Ny* by *Nz* bins. Depending on the *binstyle*, you may only specify one or two of these values; the others are effectively set to 1 (no binning in that dimension). For non-orthogonal (triclinic) simulation boxes, the bins are "tilted" slabs or pencils or bricks that are parallel to the tilted faces of the box. See the *region prism* command for a discussion of the geometry of tilted boxes in LAMMPS.

When a temperature is computed, the center-of-mass velocity for the set of atoms that are both in the compute group and in the same spatial bin is calculated. This bias velocity is then subtracted from the velocities of individual atoms in the bin to yield a thermal velocity for each atom. Note that if there is only one atom in the bin, its thermal velocity will thus be 0.0.

After the spatially-averaged velocity field has been subtracted from each atom, the temperature is calculated by the formula KE = (dim*N - dim*Nx*Ny*Nz) k T/2, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature. The dim*Nx*Ny*Nz term are degrees of freedom subtracted to adjust for the removal of the center-of-mass velocity in each of Nx*Ny*Nz bins, as discussed in the *(Evans)* paper.

If the *out* keyword is used with a *tensor* value, which is the default, a kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

If the *out* keyword is used with a *bin* value, the count of atoms and computed temperature for each bin are stored for output, as an array of values, as described below. The temperature of each bin is calculated as described above,

where the bias velocity is subtracted and only the remaining thermal velocity of atoms in the bin contributes to the temperature. See the note below for how the temperature is normalized by the degrees-of-freedom of atoms in the bin.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the *compute_modify* command if this is not the case.

The removal of the spatially-averaged velocity field by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include *fix nvt*, *fix temp/rescale*, *fix temp/berendsen*, and *fix langevin*.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as *fix shake* and *fix rigid*. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the *compute_modify* command.

Note: When using the *out* keyword with a value of *bin*, the calculated temperature for each bin does not include the degrees-of-freedom adjustment described in the preceding paragraph, for fixes that constrain molecular motion. It does include the adjustment due to the *extra* option, which is applied to each bin.

See the *Howto thermostat* doc page for a discussion of different ways to compute temperature and perform thermostatting. Using this compute in conjunction with a thermostatting fix, as explained there, will effectively implement a profile-unbiased thermostat (PUT), as described in *(Evans)*.

Output info:

This compute calculates a global scalar (the temperature). Depending on the setting of the *out* keyword, it also calculates a global vector or array. For *out* = *tensor*, it calculates a vector of length 6 (KE tensor), which can be accessed by indices 1-6. For *out* = *bin* it calculates a global array which has 2 columns and N rows, where N is the number of bins. The first column contains the number of atoms in that bin. The second contains the temperature of that bin, calculated as described above. The ordering of rows in the array is as follows. Bins in x vary fastest, then y, then z. Thus for a 10x10x10 3d array of bins, there will be 1000 rows. The bin with indices ix,iy,iz = 2,3,4 would map to row M = (iz-1)*10*10 + (iy-1)*10 + ix = 322, where the rows are numbered from 1 to 1000 and the bin indices are numbered from 1 to 10 in each dimension.

These values can be used by any command that uses global scalar or vector or array values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive". The array values are "intensive".

The scalar value will be in temperature *units*. The vector values will be in energy *units*. The first column of array values are counts; the values in the second column will be in temperature *units*.

17.130.4 Restrictions

You should not use too large a velocity-binning grid, especially in 3d. In the current implementation, the binned velocity averages are summed across all processors, so this will be inefficient if the grid is too large, and the operation is performed every timestep, as it will be for most thermostats.

17.130.5 Related commands

compute temp, *compute temp/ramp*, *compute temp/deform*, *compute pressure*

17.130.6 Default

The option default is out = tensor.

(Evans) Evans and Morriss, Phys Rev Lett, 56, 2172-2175 (1986).

17.131 compute temp/ramp command

17.131.1 Syntax

```
compute ID group-ID temp/ramp vdim vlo vhi dim clo chi keyword value ...
```

- ID, group-ID are documented in *compute* command
- temp/ramp = style name of this compute command
- vdim = *vx* or *vy* or *vz*
- vlo,vhi = subtract velocities between vlo and vhi (velocity units)
- dim = *x* or *y* or *z*
- clo,chi = lower and upper bound of domain to subtract from (distance units)
- zero or more keyword/value pairs may be appended
- keyword = *units*

units value = *lattice* or *box*

17.131.2 Examples

```
compute 2nd middle temp/ramp vx 0 8 y 2 12 units lattice
```

17.131.3 Description

Define a computation that calculates the temperature of a group of atoms, after subtracting out an ramped velocity profile before computing the kinetic energy. A compute of this style can be used by any command that computes a temperature, e.g. *thermo_modify*, *fix temp/rescale*, *fix npt*, etc.

The meaning of the arguments for this command which define the velocity ramp are the same as for the *velocity ramp* command which was presumably used to impose the velocity.

After the ramp velocity has been subtracted from the specified dimension for each atom, the temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature.

The *units* keyword determines the meaning of the distance units used for coordinates (c1,c2) and velocities (vlo,vhi). A *box* value selects standard distance units as defined by the *units* command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings; e.g. velocity = lattice spacings / tau. The *lattice* command must have been previously used to define the lattice spacing.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the *compute_modify* command if this is not the case.

The removal of the ramped velocity component by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include *fix nvt*, *fix temp/rescale*, *fix temp/berendsen*, and *fix langevin*.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as *fix shake* and *fix rigid*. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the *compute_modify* command.

See the *Howto thermostat* doc page for a discussion of different ways to compute temperature and perform thermostatting.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature *units*. The vector values will be in energy *units*.

17.131.4 Restrictions

none

17.131.5 Related commands

compute temp, *compute temp/profie*, *compute temp/deform*, *compute pressure*

17.131.6 Default

The option default is units = lattice.

17.132 compute temp/region command

17.132.1 Syntax

```
compute ID group-ID temp/region region-ID
```

- ID, group-ID are documented in *compute* command
- temp/region = style name of this compute command
- region-ID = ID of region to use for choosing atoms

17.132.2 Examples

```
compute mine flow temp/region boundary
```

17.132.3 Description

Define a computation that calculates the temperature of a group of atoms in a geometric region. This can be useful for thermostatting one portion of the simulation box. E.g. a McDLT simulation where one side is cooled, and the other side is heated. A compute of this style can be used by any command that computes a temperature, e.g. *thermo_modify*, *fix temp/rescale*, etc.

Note that a *region*-style temperature can be used to thermostat with *fix temp/rescale* or *fix langevin*, but should probably not be used with Nose/Hoover style fixes (*fix nvt*, *fix npt*, or *fix nph*), if the degrees-of-freedom included in the computed T varies with time.

The temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in both the group and region, k = Boltzmann constant, and T = temperature.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is calculated each time the temperature is evaluated since it is assumed atoms can enter/leave the region. Thus there is no need to use the *dynamic* option of the *compute_modify* command for this compute style.

The removal of atoms outside the region by this fix is essentially computing the temperature after a "bias" has been removed, which in this case is the velocity of any atoms outside the region. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include *fix nvt*, *fix temp/rescale*, *fix temp/berendsen*, and *fix langevin*. This means that when this compute is used to calculate the temperature for any of the thermostatting fixes via the *fix modify temp* command, the thermostat will operate only on atoms that are currently in the geometric region.

Unlike other compute styles that calculate temperature, this compute does not subtract out degrees-of-freedom due to fixes that constrain motion, such as *fix shake* and *fix rigid*. This is because those degrees of freedom (e.g. a constrained bond) could apply to sets of atoms that straddle the region boundary, and hence the concept is somewhat ill-defined. If needed the number of subtracted degrees-of-freedom can be set explicitly using the *extra* option of the *compute_modify* command.

See the *Howto thermostat* doc page for a discussion of different ways to compute temperature and perform thermostatting.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature *units*. The vector values will be in energy *units*.

17.132.4 Restrictions

none

17.132.5 Related commands

compute temp, *compute pressure*

Default: none

17.133 compute temp/region/eff command

17.133.1 Syntax

```
compute ID group-ID temp/region/eff region-ID
```

- ID, group-ID are documented in *compute* command
- temp/region/eff = style name of this compute command
- region-ID = ID of region to use for choosing atoms

17.133.2 Examples

```
compute mine flow temp/region/eff boundary
```

17.133.3 Description

Define a computation that calculates the temperature of a group of nuclei and electrons in the *electron force field* model, within a geometric region using the electron force field. A compute of this style can be used by commands that compute a temperature, e.g. *thermo_modify*.

The operation of this compute is exactly like that described by the *compute temp/region* command, except that the formula for the temperature itself includes the radial electron velocity contributions, as discussed by the *compute temp/eff* command.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature *units*. The vector values will be in energy *units*.

17.133.4 Restrictions

This compute is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.133.5 Related commands

compute temp/region, *compute temp/eff*, *compute pressure*

Default: none

17.134 compute temp/rotate command

17.134.1 Syntax

```
compute ID group-ID temp/rotate
```

- ID, group-ID are documented in *compute* command
- temp/rotate = style name of this compute command

17.134.2 Examples

```
compute Tbead bead temp/rotate
```

17.134.3 Description

Define a computation that calculates the temperature of a group of atoms, after subtracting out the center-of-mass velocity and angular velocity of the group. This is useful if the group is expected to have a non-zero net velocity and/or global rotation motion for some reason. A compute of this style can be used by any command that computes a temperature, e.g. *thermo_modify*, *fix temp/rescale*, *fix npt*, etc.

After the center-of-mass velocity and angular velocity has been subtracted from each atom, the temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the *compute_modify* command if this is not the case.

The removal of the center-of-mass velocity and angular velocity by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include *fix nvt*, *fix temp/rescale*, *fix temp/berendsen*, and *fix langevin*.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as *fix shake* and *fix rigid*. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the *compute_modify* command.

See the *Howto thermostat* doc page for a discussion of different ways to compute temperature and perform thermostatting.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature *units*. The vector values will be in energy *units*.

17.134.4 Restrictions

This compute is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.134.5 Related commands

compute temp

Default: none

17.135 compute temp/sphere command

17.135.1 Syntax

```
compute ID group-ID temp/sphere keyword value ...
```

- ID, group-ID are documented in *compute* command
- temp/sphere = style name of this compute command
- zero or more keyword/value pairs may be appended
- keyword = *bias* or *dof*

```
bias value = bias-ID
  bias-ID = ID of a temperature compute that removes a velocity bias
dof value = all or rotate
  all = compute temperature of translational and rotational degrees of␣
↪freedom
  rotate = compute temperature of just rotational degrees of freedom
```

17.135.2 Examples

```
compute 1 all temp/sphere
compute myTemp mobile temp/sphere bias tempCOM
compute myTemp mobile temp/sphere dof rotate
```

17.135.3 Description

Define a computation that calculates the temperature of a group of spherical particles, including a contribution from both their translational and rotational kinetic energy. This differs from the usual *compute temp* command, which assumes point particles with only translational kinetic energy.

Both point and finite-size particles can be included in the group. Point particles do not rotate, so they have only 3 translational degrees of freedom. For 3d spherical particles, each has 6 degrees of freedom (3 translational, 3 rotational). For 2d spherical particles, each has 3 degrees of freedom (2 translational, 1 rotational).

Note: This choice for degrees of freedom (dof) assumes that all finite-size spherical particles in your model will freely rotate, sampling all their rotational dof. It is possible to use a combination of interaction potentials and fixes that induce no torque or otherwise constrain some of all of your particles so that this is not the case. Then there are less dof and you should use the *compute_modify extra* command to adjust the dof accordingly.

The translational kinetic energy is computed the same as is described by the *compute temp* command. The rotational kinetic energy is computed as 1/2 I w^2, where I is the moment of inertia for a sphere and w is the particle's angular velocity.

Note: For *2d models*, particles are treated as spheres, not disks, meaning their moment of inertia will be the same as in 3d.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute. The formula for the components of the tensor is the same as the above formulas, except that v^2 and w^2 are replaced by vx*vy and wx*wy for the xy component. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the *compute_modify* command if this is not the case.

This compute subtracts out translational degrees-of-freedom due to fixes that constrain molecular motion, such as *fix shake* and *fix rigid*. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the *compute_modify* command.

See the *Howto thermostat* doc page for a discussion of different ways to compute temperature and perform thermostatting.

The keyword/value option pairs are used in the following ways.

For the *bias* keyword, *bias-ID* refers to the ID of a temperature compute that removes a "bias" velocity from each atom. This allows compute temp/sphere to compute its thermal temperature after the translational kinetic energy components have been altered in a prescribed way, e.g. to remove a flow velocity profile. Thermostats that use this compute will work with this bias term. See the doc pages for individual computes that calculate a temperature and the doc pages for fixes that perform thermostatting for more details.

For the *dof* keyword, a setting of *all* calculates a temperature that includes both translational and rotational degrees of freedom. A setting of *rotate* calculates a temperature that includes only rotational degrees of freedom.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature *units*. The vector values will be in energy *units*.

17.135.4 Restrictions

This fix requires that atoms store torque and angular velocity (omega) and a radius as defined by the *atom_style sphere* command.

All particles in the group must be finite-size spheres, or point particles with radius = 0.0.

17.135.5 Related commands

compute temp, *compute temp/asphere*

17.135.6 Default

The option defaults are no bias and dof = all.

17.136 compute temp/uef command

17.136.1 Syntax

```
compute ID group-ID temp/uef
```

- ID, group-ID are documented in *compute* command
- temp/uef = style name of this compute command

17.136.2 Examples

```
compute 1 all temp/uef
compute 2 sel temp/uef
```

17.136.3 Description

This command is used to compute the kinetic energy tensor in the reference frame of the applied flow field when *fix nvt/uef* or *fix npt/uef* is used. It is not necessary to use this command to compute the scalar value of the temperature. A *compute temp* may be used for that purpose.

Output information for this command can be found in the documentation for *compute temp*.

17.136.4 Restrictions

This fix is part of the USER-UEF package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This command can only be used when *fix nvt/uef* or *fix npt/uef* is active.

17.136.5 Related commands

compute temp, *fix nvt/uef*, *compute pressure/uef*

Default: none

17.137 compute ti command

17.137.1 Syntax

```
compute ID group ti keyword args ...
```

- ID, group-ID are documented in *compute* command
- ti = style name of this compute command
- one or more attribute/arg pairs may be appended
- keyword = pair style (lj/cut, gauss, born, etc) or *tail* or *kspace*

```
pair style args = atype v_name1 v_name2
  atype = atom type (see asterisk form below)
  v_name1 = variable with name1 that is energy scale factor and function␣
↪of lambda
  v_name2 = variable with name2 that is derivative of v_name1 with␣
↪respect to lambda
tail args = atype v_name1 v_name2
  atype = atom type (see asterisk form below)
  v_name1 = variable with name1 that is energy tail correction scale␣
↪factor and function of lambda
  v_name2 = variable with name2 that is derivative of v_name1 with␣
↪respect to lambda
kspace args = atype v_name1 v_name2
  atype = atom type (see asterisk form below)
  v_name1 = variable with name1 that is K-Space scale factor and function␣
↪of lambda
  v_name2 = variable with name2 that is derivative of v_name1 with␣
↪respect to lambda
```

17.137.2 Examples

```
compute 1 all ti lj/cut 1 v_lj v_dlj coul/long 2 v_c v_dc kspace 1 v_ks v_dks
compute 1 all ti lj/cut 1*3 v_lj v_dlj coul/long * v_c v_dc kspace * v_ks v_
↪dks
```

17.137.3 Description

Define a computation that calculates the derivative of the interaction potential with respect to *lambda*, the coupling parameter used in a thermodynamic integration. This derivative can be used to infer a free energy difference resulting from an alchemical simulation, as described in *Eike*.

Typically this compute will be used in conjunction with the *fix adapt* command which can perform alchemical transformations by adjusting the strength of an interaction potential as a simulation runs, as defined by one or more *pair_style* or *kspace_style* commands. This scaling is done via a prefactor on the energy, forces, virial calculated by the pair or K-Space style. The prefactor is often a function of a *lambda* parameter which may be adjusted from 0 to 1 (or vice versa) over the course of a *run*. The time-dependent adjustment is what the *fix adapt* command does.

Assume that the unscaled energy of a pair_style or kspace_style is given by U. Then the scaled energy is

```
Us = f(lambda) U
```

where f() is some function of lambda. What this compute calculates is

```
dUs / d(lambda) = U df(lambda)/dlambda = Us / f(lambda) df(lambda)/dlambda
```

which is the derivative of the system's scaled potential energy Us with respect to *lambda*.

To perform this calculation, you provide one or more atom types as *atype*. *Atype* can be specified in one of two ways. An explicit numeric values can be used, as in the 1st example above. Or a wildcard asterisk can be used in place of or in conjunction with the *atype* argument to select multiple atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

You also specify two functions, as *equal-style variables*. The first is specified as *v_name1*, where *name1* is the name of the variable, and is f(lambda) in the notation above. The second is specified as *v_name2*, where *name2* is the name of the variable, and is df(lambda) / dlambda in the notation above. I.e. it is the analytic derivative of f() with respect to lambda. Note that the *name1* variable is also typically given as an argument to the *fix adapt* command.

An alchemical simulation may use several pair potentials together, invoked via the *pair_style hybrid or hybrid/overlay* command. The total dUs/dlambda for the overall system is calculated as the sum of each contributing term as listed by the keywords in the compute ti command. Individual pair potentials can be listed, which will be sub-styles in the hybrid case. You can also include a K-space term via the *kspace* keyword. You can also include a pairwise long-range tail correction to the energy via the *tail* keyword.

For each term you can specify a different (or the same) scale factor by the two variables that you list. Again, these will typically correspond toe the scale factors applied to these various potentials and the K-Space contribution via the *fix adapt* command.

More details about the exact functional forms for the computation of du/dl can be found in the paper by *Eike*.

Output info:

This compute calculates a global scalar, namely dUs/dlambda. This value can be used by any command that uses a global scalar value from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive".

The scalar value will be in energy *units*.

17.137.4 Restrictions

This compute is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

17.137.5 Related commands

fix adapt

Default: none

(Eike) Eike and Maginn, Journal of Chemical Physics, 124, 164503 (2006).

17.138 compute torque/chunk command

17.138.1 Syntax

```
compute ID group-ID torque/chunk chunkID
```

- ID, group-ID are documented in *compute* command
- torque/chunk = style name of this compute command
- chunkID = ID of *compute chunk/atom* command

17.138.2 Examples

```
compute 1 fluid torque/chunk molchunk
```

17.138.3 Description

Define a computation that calculates the torque on multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a *compute chunk/atom* command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the *compute chunk/atom* and *Howto chunk* doc pages for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

This compute calculates the 3 components of the torque vector for eqch chunk, due to the forces on the individual atoms in the chunk around the center-of-mass of the chunk. The calculation includes all effects due to atoms passing through periodic boundaries.

Note that only atoms in the specified group contribute to the calculation. The *compute chunk/atom* command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

Note: The coordinates of an atom contribute to the chunk's torque in "unwrapped" form, by using the image flags associated with each atom. See the *dump custom* command for a discussion of "unwrapped" coordinates. See the Atoms section of the *read_data* command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the *set image* command.

The simplest way to output the results of the compute torque/chunk calculation to a file is to use the *fix ave/time* command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all torque/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk[*] file tmp.out mode vector
```

Output info:

This compute calculates a global array where the number of rows = the number of chunks *Nchunk* as calculated by the specified *compute chunk/atom* command. The number of columns = 3 for the 3 xyz components of the torque for each chunk. These values can be accessed by any command that uses global array values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The array values are "intensive". The array values will be in force-distance *units*.

17.138.4 Restrictions

none

17.138.5 Related commands

variable torque() function

Default: none

17.139 compute vacf command

17.139.1 Syntax

```
compute ID group-ID vacf
```

- ID, group-ID are documented in *compute* command
- vacf = style name of this compute command

17.139.2 Examples

```
compute 1 all vacf
compute 1 upper vacf
```

17.139.3 Description

Define a computation that calculates the velocity auto-correlation function (VACF), averaged over a group of atoms. Each atom's contribution to the VACF is its current velocity vector dotted into its initial velocity vector at the time the compute was specified.

A vector of four quantities is calculated by this compute. The first 3 elements of the vector are vx * vx0 (and similarly for the y and z components), summed and averaged over atoms in the group. Vx is the current x-component of velocity for the atom, vx0 is the initial x-component of velocity for the atom. The 4th element of the vector is the total VACF, i.e. (vx*vx0 + vy*vy0 + vz*vz0), summed and averaged over atoms in the group.

The integral of the VACF versus time is proportional to the diffusion coefficient of the diffusing atoms. This can be computed in the following manner, using the *variable trap()* function:

```
compute         2 all vacf
fix             5 all vector 1 c_2[4]
variable        diff equal dt*trap(f_5)
thermo_style    custom step v_diff
```

Note: If you want the quantities calculated by this compute to be continuous when running from a *restart file*, then you should use the same ID for this compute, as in the original run. This is so that the fix this compute creates to store per-atom quantities will also have the same ID, and thus be initialized correctly with time=0 atom velocities from the restart file.

Output info:

This compute calculates a global vector of length 4, which can be accessed by indices 1-4 by any command that uses global vector values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The vector values are "intensive". The vector values will be in velocity^2 *units*.

17.139.4 Restrictions

none

17.139.5 Related commands

compute msd

Default: none

17.140 compute vcm/chunk command

17.140.1 Syntax

```
compute ID group-ID vcm/chunk chunkID
```

- ID, group-ID are documented in *compute* command
- vcm/chunk = style name of this compute command
- chunkID = ID of *compute chunk/atom* command

17.140.2 Examples

```
compute 1 fluid vcm/chunk molchunk
```

17.140.3 Description

Define a computation that calculates the center-of-mass velocity for multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a *compute chunk/atom* command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the *compute chunk/atom* and *Howto chunk* doc pages for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

This compute calculates the x,y,z components of the center-of-mass velocity for each chunk. This is done by summing mass*velocity for each atom in the chunk and dividing the sum by the total mass of the chunk.

Note that only atoms in the specified group contribute to the calculation. The *compute chunk/atom* command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

The simplest way to output the results of the compute vcm/chunk calculation to a file is to use the *fix ave/time* command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all vcm/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk[*] file tmp.out mode vector
```

Output info:

This compute calculates a global array where the number of rows = the number of chunks *Nchunk* as calculated by the specified *compute chunk/atom* command. The number of columns = 3 for the x,y,z center-of-mass velocity coordinates of each chunk. These values can be accessed by any command that uses global array values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

The array values are "intensive". The array values will be in velocity *units*.

17.140.4 Restrictions

none

Related commands: none

Default: none

17.141 compute voronoi/atom command

17.141.1 Syntax

```
compute ID group-ID voronoi/atom keyword arg ...
```

- ID, group-ID are documented in *compute* command
- voronoi/atom = style name of this compute command

- zero or more keyword/value pairs may be appended
- keyword = *only_group* or *surface* or *radius* or *edge_histo* or *edge_threshold* or *face_threshold* or *neighbors* or *peratom*

```
only_group = no arg
occupation = no arg
surface arg = sgroup-ID
  sgroup-ID = compute the dividing surface between group-ID and sgroup-ID
    this keyword adds a third column to the compute output
radius arg = v_r
  v_r = radius atom style variable for a poly-disperse Voronoi␣
↪tessellation
edge_histo arg = maxedge
  maxedge = maximum number of Voronoi cell edges to be accounted in the␣
↪histogram
edge_threshold arg = minlength
  minlength = minimum length for an edge to be counted
face_threshold arg = minarea
  minarea = minimum area for a face to be counted
neighbors value = yes or no = store list of all neighbors or no
peratom value = yes or no = per-atom quantities accessible or no
```

17.141.2 Examples

```
compute 1 all voronoi/atom
compute 2 precipitate voronoi/atom surface matrix
compute 3b precipitate voronoi/atom radius v_r
compute 4 solute voronoi/atom only_group
compute 5 defects voronoi/atom occupation
compute 6 all voronoi/atom neighbors yes
```

17.141.3 Description

Define a computation that calculates the Voronoi tessellation of the atoms in the simulation box. The tessellation is calculated using all atoms in the simulation, but non-zero values are only stored for atoms in the group.

By default two per-atom quantities are calculated by this compute. The first is the volume of the Voronoi cell around each atom. Any point in an atom's Voronoi cell is closer to that atom than any other. The second is the number of faces of the Voronoi cell. This is equal to the number of nearest neighbors of the central atom, plus any exterior faces (see note below). If the *peratom* keyword is set to "no", the per-atom quantities are still calculated, but they are not accessible.

If the *only_group* keyword is specified the tessellation is performed only with respect to the atoms contained in the compute group. This is equivalent to deleting all atoms not contained in the group prior to evaluating the tessellation.

If the *surface* keyword is specified a third quantity per atom is computed: the Voronoi cell surface of the given atom. *surface* takes a group ID as an argument. If a group other than *all* is specified, only the Voronoi cell facets facing a neighbor atom from the specified group are counted towards the surface area.

In the example above, a precipitate embedded in a matrix, only atoms at the surface of the precipitate will have non-zero surface area, and only the outward facing facets of the Voronoi cells are counted (the hull of the precipitate). The total surface area of the precipitate can be obtained by running a "reduce sum" compute on c_2[3]

If the *radius* keyword is specified with an atom style variable as the argument, a poly-disperse Voronoi tessellation is performed. Examples for radius variables are

```
variable r1 atom (type==1)*0.1+(type==2)*0.4
compute radius all property/atom radius
variable r2 atom c_radius
```

Here v_r1 specifies a per-type radius of 0.1 units for type 1 atoms and 0.4 units for type 2 atoms, and v_r2 accesses the radius property present in atom_style sphere for granular models.

The *edge_histo* keyword activates the compilation of a histogram of number of edges on the faces of the Voronoi cells in the compute group. The argument *maxedge* of the this keyword is the largest number of edges on a single Voronoi cell face expected to occur in the sample. This keyword adds the generation of a global vector with *maxedge*+1 entries. The last entry in the vector contains the number of faces with more than *maxedge* edges. Since the polygon with the smallest amount of edges is a triangle, entries 1 and 2 of the vector will always be zero.

The *edge_threshold* and *face_threshold* keywords allow the suppression of edges below a given minimum length and faces below a given minimum area. Ultra short edges and ultra small faces can occur as artifacts of the Voronoi tessellation. These keywords will affect the neighbor count and edge histogram outputs.

If the *occupation* keyword is specified the tessellation is only performed for the first invocation of the compute and then stored. For all following invocations of the compute the number of atoms in each Voronoi cell in the stored tessellation is counted. In this mode the compute returns a per-atom array with 2 columns. The first column is the number of atoms currently in the Voronoi volume defined by this atom at the time of the first invocation of the compute (note that the atom may have moved significantly). The second column contains the total number of atoms sharing the Voronoi cell of the stored tessellation at the location of the current atom. Numbers in column one can be any positive integer including zero, while column two values will always be greater than zero. Column one data can be used to locate vacancies (the coordinates are given by the atom coordinates at the time step when the compute was first invoked), while column two data can be used to identify interstitial atoms.

If the *neighbors* value is set to yes, then this compute creates a local array with 3 columns. There is one row for each face of each Voronoi cell. The 3 columns are the atom ID of the atom that owns the cell, the atom ID of the atom in the neighboring cell (or zero if the face is external), and the area of the face. The array can be accessed by any command that uses local values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options. More specifically, the array can be accessed by a *dump local* command to write a file containing all the Voronoi neighbors in a system:

```
compute 6 all voronoi/atom neighbors yes
dump d2 all local 1 dump.neighbors index c_6[1] c_6[2] c_6[3]
```

If the *face_threshold* keyword is used, then only faces with areas greater than the threshold are stored.

The Voronoi calculation is performed by the freely available Voro++ package, written by Chris Rycroft at UC Berkeley and LBL, which must be installed on your system when building LAMMPS for use with this compute. See instructions on obtaining and installing the Voro++ software in the src/VORONOI/README file.

Note: The calculation of Voronoi volumes is performed by each processor for the atoms it owns, and includes the effect of ghost atoms stored by the processor. This assumes that the Voronoi cells of owned atoms are not affected by atoms beyond the ghost atom cut-off distance. This is usually a good assumption for liquid and solid systems, but may lead to underestimation of Voronoi volumes in low density systems. By default, the set of ghost atoms stored by each processor is determined by the cutoff used for *pair_style* interactions. The cutoff can be set explicitly via the *comm_modify cutoff* command. The Voronoi cells for atoms adjacent to empty regions will extend into those regions up to the communication cutoff in x, y, or z. In that situation, an exterior face is created at the cutoff distance normal to the x, y, or z direction. For triclinic systems, the exterior face is parallel to the corresponding reciprocal lattice vector.

Note: The Voro++ package performs its calculation in 3d. This will still work for a 2d LAMMPS simulation, provided all the atoms have the same z coordinate. The Voronoi cell of each atom will be a columnar polyhedron with constant cross-sectional area along the z direction and two exterior faces at the top and bottom of the simulation box. If the atoms do not all have the same z coordinate, then the columnar cells will be accordingly distorted. The cross-sectional area of each Voronoi cell can be obtained by dividing its volume by the z extent of the simulation box. Note that you define the z extent of the simulation box for 2d simulations when using the *create_box* or *read_data* commands.

Output info:

By default, this compute calculates a per-atom array with 2 columns. In regular dynamic tessellation mode the first column is the Voronoi volume, the second is the neighbor count, as described above (read above for the output data in case the *occupation* keyword is specified). These values can be accessed by any command that uses per-atom values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options. If the *peratom* keyword is set to "no", the per-atom array is still created, but it is not accessible.

If the *edge_histo* keyword is used, then this compute generates a global vector of length *maxedge*+1, containing a histogram of the number of edges per face.

If the *neighbors* value is set to yes, then this compute calculates a local array with 3 columns. There is one row for each face of each Voronoi cell.

Note: Some LAMMPS commands such as the *compute reduce* command can accept either a per-atom or local quantity. If this compute produces both quantities, the command may access the per-atom quantity, even if you want to access the local quantity. This effect can be eliminated by using the *peratom* keyword to turn off the production of the per-atom quantities. For the default value *yes* both quantities are produced. For the value *no*, only the local array is produced.

The Voronoi cell volume will be in distance *units* cubed. The Voronoi face area will be in distance *units* squared.

17.141.4 Restrictions

This compute is part of the VORONOI package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

It also requires you have a copy of the Voro++ library built and installed on your system. See instructions on obtaining and installing the Voro++ software in the src/VORONOI/README file.

17.141.5 Related commands

dump custom, *dump local*

Default: *neighbors* no, *peratom* yes

17.142 compute xrd command

17.142.1 Syntax

```
compute ID group-ID xrd lambda type1 type2 ... typeN keyword value ...
```

- ID, group-ID are documented in *compute* command
- xrd = style name of this compute command
- lambda = wavelength of incident radiation (length units)
- type1 type2 ... typeN = chemical symbol of each atom type (see valid options below)
- zero or more keyword/value pairs may be appended
- keyword = *2Theta* or *c* or *LP* or *manual* or *echo*

```
2Theta values = Min2Theta Max2Theta
  Min2Theta,Max2Theta = minimum and maximum 2 theta range to explore
  (radians or degrees)
c values = c1 c2 c3
  c1,c2,c3 = parameters to adjust the spacing of the reciprocal
             lattice nodes in the h, k, and l directions respectively
LP value = switch to apply Lorentz-polarization factor
  0/1 = off/on
manual = flag to use manual spacing of reciprocal lattice points
           based on the values of the c parameters
echo = flag to provide extra output for debugging purposes
```

17.142.2 Examples

```
compute 1 all xrd 1.541838 Al O 2Theta 0.087 0.87 c 1 1 1 LP 1 echo
compute 2 all xrd 1.541838 Al O 2Theta 10 100 c 0.05 0.05 0.05 LP 1 manual

fix 1 all ave/histo/weight 1 1 1 0.087 0.87 250 c_1[1] c_1[2] mode vector file␣
↪Rad2Theta.xrd
fix 2 all ave/histo/weight 1 1 1 10 100 250 c_2[1] c_2[2] mode vector file Deg2Theta.
↪xrd
```

17.142.3 Description

Define a computation that calculates x-ray diffraction intensity as described in *(Coleman)* on a mesh of reciprocal lattice nodes defined by the entire simulation domain (or manually) using a simulated radiation of wavelength lambda.

The x-ray diffraction intensity, I, at each reciprocal lattice point, k, is computed from the structure factor, F, using the

equations:

$$
\begin{aligned}
I =& Lp(\theta)\frac{F^*F}{N} \\
F(\mathbf{k}) =& \sum_{j=1}^{N} f_j(\theta)exp(2\pi i\mathbf{k}\cdot\mathbf{r}_j) \\
Lp(\theta) =& \frac{1+cos^2(2\theta)}{cos(\theta)sin^2(\theta)} \\
\frac{sin(\theta)}{\lambda} =& \frac{|\mathbf{k}|}{2}
\end{aligned}
$$

Here, K is the location of the reciprocal lattice node, r_j is the position of each atom, f_j are atomic scattering factors, *Lp* is the Lorentz-polarization factor, and θ is the scattering angle of diffraction. The Lorentz-polarization factor can be turned off using the optional *LP* keyword.

Diffraction intensities are calculated on a three-dimensional mesh of reciprocal lattice nodes. The mesh spacing is defined either (a) by the entire simulation domain or (b) manually using selected values as shown in the 2D diagram below.

For a mesh defined by the simulation domain, a rectilinear grid is constructed with spacing *c**inv(A) along each reciprocal lattice axis. Where A are the vectors corresponding to the edges of the simulation cell. If one or two directions has non-periodic boundary conditions, then the spacing in these directions is defined from the average of the (inversed) box lengths with periodic boundary conditions. Meshes defined by the simulation domain must contain at least one periodic boundary.

If the *manual* flag is included, the mesh of reciprocal lattice nodes will defined using the *c* values for the spacing along each reciprocal lattice axis. Note that manual mapping of the reciprocal space mesh is good for comparing diffraction results from multiple simulations; however it can reduce the likelihood that Bragg reflections will be satisfied unless small spacing parameters (< 0.05 Angstrom^(-1)) are implemented. Meshes with manual spacing do not require a periodic boundary.

The limits of the reciprocal lattice mesh are determined by range of scattering angles explored. The *2Theta* parameters allows the user to reduce the scattering angle range to only the region of interest which reduces the cost of the computation.

The atomic scattering factors, fj, accounts for the reduction in diffraction intensity due to Compton scattering. Compute xrd uses analytical approximations of the atomic scattering factors that vary for each atom type (type1 type2 ... typeN) and angle of diffraction. The analytic approximation is computed using the formula *(Colliex)*:

$$
f_j\left(\frac{sin(\theta)}{\lambda}\right) = \sum_{i}^{4} a_i exp\left(-b_i\frac{sin^2(\theta)}{\lambda^2}\right) + c
$$

Coefficients parameterized by *(Peng)* are assigned for each atom type designating the chemical symbol and charge of each atom type. Valid chemical symbols for compute xrd are:

H	He1-	He	Li	Li1+
Be	Be2+	B	C	Cval
N	O	O1-	F	F1-
Ne	Na	Na1+	Mg	Mg2+
Al	Al3+	Si	Sival	Si4+
P	S	Cl	Cl1-	Ar
K	Ca	Ca2+	Sc	Sc3+
Ti	Ti2+	Ti3+	Ti4+	V

Continued on next page

Table 1 – continued from previous page

V2+	V3+	V5+	Cr	Cr2+
Cr3+	Mn	Mn2+	Mn3+	Mn4+
Fe	Fe2+	Fe3+	Co	Co2+
Co	Ni	Ni2+	Ni3+	Cu
Cu1+	Cu2+	Zn	Zn2+	Ga
Ga3+	Ge	Ge4+	As	Se
Br	Br1-	Kr	Rb	Rb1+
Sr	Sr2+	Y	Y3+	Zr
Zr4+	Nb	Nb3+	Nb5+	Mo
Mo3+	Mo5+	Mo6+	Tc	Ru
Ru3+	Ru4+	Rh	Rh3+	Rh4+
Pd	Pd2+	Pd4+	Ag	Ag1+
Ag2+	Cd	Cd2+	In	In3+
Sn	Sn2+	Sn4+	Sb	Sb3+
Sb5+	Te	I	I1-	Xe
Cs	Cs1+	Ba	Ba2+	La
La3+	Ce	Ce3+	Ce4+	Pr
Pr3+	Pr4+	Nd	Nd3+	Pm
Pm3+	Sm	Sm3+	Eu	Eu2+
Eu3+	Gd	Gd3+	Tb	Tb3+
Dy	Dy3+	Ho	Ho3+	Er
Er3+	Tm	Tm3+	Yb	Yb2+
Yb3+	Lu	Lu3+	Hf	Hf4+
Ta	Ta5+	W	W6+	Re
Os	Os4+	Ir	Ir3+	Ir4+
Pt	Pt2+	Pt4+	Au	Au1+
Au3+	Hg	Hg1+	Hg2+	Tl
Tl1+	Tl3+	Pb	Pb2+	Pb4+
Bi	Bi3+	Bi5+	Po	At
Rn	Fr	Ra	Ra2+	Ac
Ac3+	Th	Th4+	Pa	U
U3+	U4+	U6+	Np	Np3+
Np4+	Np6+	Pu	Pu3+	Pu4+
Pu6+	Am	Cm	Bk	Cf

If the *echo* keyword is specified, compute xrd will provide extra reporting information to the screen.

Output info:

This compute calculates a global array. The number of rows in the array is the number of reciprocal lattice nodes that are explored which by the mesh. The global array has 2 columns.

The first column contains the diffraction angle in the units (radians or degrees) provided with the *2Theta* values. The second column contains the computed diffraction intensities as described above.

The array can be accessed by any command that uses global values from a compute as input. See the *Howto output* doc page for an overview of LAMMPS output options.

All array values calculated by this compute are "intensive".

17.142.4 Restrictions

This compute is part of the USER-DIFFRACTION package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

The compute_xrd command does not work for triclinic cells.

17.142.5 Related commands

fix ave/histo, *compute saed*

17.142.6 Default

The option defaults are 2Theta = 1 179 (degrees), c = 1 1 1, LP = 1, no manual flag, no echo flag.

(Coleman) Coleman, Spearot, Capolungo, MSMSE, 21, 055020 (2013).

(Colliex) Colliex et al. International Tables for Crystallography Volume C: Mathematical and Chemical Tables, 249-429 (2004).

(Peng) Peng, Ren, Dudarev, Whelan, Acta Crystallogr. A, 52, 257-76 (1996).

CHAPTER

EIGHTEEN

PAIR STYLES

18.1 pair_style adp command

18.2 pair_style adp/omp command

18.2.1 Syntax

```
pair_style adp
```

18.2.2 Examples

```
pair_style adp
pair_coeff * * Ta.adp Ta
pair_coeff * * ../potentials/AlCu.adp Al Al Cu
```

18.2.3 Description

Style *adp* computes pairwise interactions for metals and metal alloys using the angular dependent potential (ADP) of *(Mishin)*, which is a generalization of the *embedded atom method (EAM) potential*. The LAMMPS implementation is discussed in *(Singh)*. The total energy Ei of an atom I is given by

$$
\begin{aligned}
E_i &= F_\alpha\left(\sum_{j\neq i}\rho_\beta(r_{ij})\right) + \frac{1}{2}\sum_{j\neq i}\phi_{\alpha\beta}(r_{ij}) + \frac{1}{2}\sum_s(\mu_i^s)^2 + \frac{1}{2}\sum_{s,t}(\lambda_i^{st})^2 - \frac{1}{6}\nu_i^2 \\
\mu_i^s &= \sum_{j\neq i} u_{\alpha\beta}(r_{ij})r_{ij}^s \\
\lambda_i^{st} &= \sum_{j\neq i} w_{\alpha\beta}(r_{ij})r_{ij}^s r_{ij}^t \\
\nu_i &= \sum_s \lambda_i^{ss}
\end{aligned}
$$

where F is the embedding energy which is a function of the atomic electron density ρ, ϕ is a pair potential interaction, α and β are the element types of atoms I and J, and s and $t = 1, 2, 3$ and refer to the cartesian coordinates. The μ and λ terms represent the dipole and quadruple distortions of the local atomic environment which extend the original EAM framework by introducing angular forces.

Note that unlike for other potentials, cutoffs for ADP potentials are not set in the pair_style or pair_coeff command; they are specified in the ADP potential files themselves. Likewise, the ADP potential files list atomic masses; thus you do not need to use the *mass* command to specify them.

ADP potentials are available from:

- The NIST WWW site at http://www.ctcms.nist.gov/potentials. Note that ADP potentials obtained from NIST must be converted into the extended DYNAMO *setfl* format discussed below.
- The OpenKIM Project at https://openkim.org/browse/models/by-type provides ADP potentials that can be used directly in LAMMPS with the *kim_commands interface*.

Only a single pair_coeff command is used with the *adp* style which specifies an extended DYNAMO *setfl* file, which contains information for M elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of extended *setfl* elements to atom types

See the *pair_coeff* doc page for alternate ways to specify the path for the potential file.

As an example, the potentials/AlCu.adp file, included in the potentials directory of the LAMMPS distribution, is an extended *setfl* file which has tabulated ADP values for w elements and their alloy interactions: Cu and Al. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Al, and the 4th to be Cu, you would use the following pair_coeff command:

```
pair_coeff * * AlCu.adp Al Al Al Cu
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Al arguments map LAMMPS atom types 1,2,3 to the Al element in the extended *setfl* file. The final Cu argument maps LAMMPS atom type 4 to the Al element in the extended *setfl* file. Note that there is no requirement that your simulation use all the elements specified by the extended *setfl* file.

If a mapping value is specified as NULL, the mapping is not performed. This can be used when an *adp* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Adp files in the *potentials* directory of the LAMMPS distribution have an ".adp" suffix. A DYNAMO *setfl* file extended for ADP is formatted as follows. Basically it is the standard *setfl* format with additional tabulated functions u and w added to the file after the tabulated pair potentials. See the *pair_eam* command for further details on the *setfl* format.

- lines 1,2,3 = comments (ignored)
- line 4: N_{elements} Element1 Element2 ... ElementN
- line 5: N_ρ, d_ρ, N_r, d_r, cutoff

Following the 5 header lines are N_{elements} sections, one for each element, each with the following format:

- line 1 = atomic number, mass, lattice constant, lattice type (e.g. FCC)
- embedding function $F(\rho)$ (N_ρ values)
- density function $\rho(r)$ (N_r values)

Following the N_{elements} sections, N_r values for each pair potential $\phi(r)$ array are listed for all i, j element pairs in the same format as other arrays. Since these interactions are symmetric ($i, j = j, i$) only ϕ arrays with $i \geq j$ are listed, in the following order:

$$i, j = (1,1), (2,1), (2,2), (3,1), (3,2), (3,3), (4,1), ..., (N_{\text{elements}}, N_{\text{elements}}).$$

The tabulated values for each ϕ function are listed as $r * \phi$ (in units of eV-Angstroms), since they are for atom pairs, the same as for *other EAM files*.

After the $\phi(r)$ arrays, each of the $u(r)$ arrays are listed in the same order with the same assumptions of symmetry. Directly following the $u(r)$, the $w(r)$ arrays are listed. Note that $\phi(r)$ is the only array tabulated with a scaling by r.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, no special mixing rules are needed, since the ADP potential files specify alloy interactions explicitly.

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in tabulated potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.2.4 Restrictions

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package.

18.2.5 Related commands

pair_coeff, *pair_eam*

Default: none

(Mishin) Mishin, Mehl, and Papaconstantopoulos, Acta Mater, 53, 4029 (2005).

(Singh) Singh and Warner, Acta Mater, 58, 5797-5805 (2010),

18.3 pair_style agni command

18.4 pair_style agni/omp command

18.4.1 Syntax

```
pair_style agni
```

18.4.2 Examples

```
pair_style      agni
pair_coeff      * * Al.agni Al
```

18.4.3 Description

Style *agni* style computes the many-body vectorial force components for an atom as

$$F_i^u = \sum_t^{N_t} \alpha_t \cdot \exp\left[-\frac{\left(d_{i,t}^u\right)^2}{2l^2}\right]$$
$$d_{i,t}^u = ||V_i^u(\eta) - V_t^u(\eta)||$$
$$V_i^u(\eta) = \sum_{j \neq i} \frac{r_{ij}^u}{r_{ij}} \cdot e^{-\left(\frac{r_{ij}}{\eta}\right)^2} \cdot f_d\left(r_{ij}\right)$$
$$f_d\left(r_{ij}\right) = \frac{1}{2}\left[\cos\left(\frac{\pi r_{ij}}{R_c}\right) + 1\right]$$

u labels the individual components, i.e. x, y or z, and V is the corresponding atomic fingerprint. d is the Euclidean distance between any two atomic fingerprints. A total of N_t reference atomic environments are considered to construct the force field file. α_t and l are the weight coefficients and length scale parameter of the non-linear regression model.

The method implements the recently proposed machine learning access to atomic forces as discussed extensively in the following publications - *(Botu1)* and *(Botu2)*. The premise of the method is to map the atomic environment numerically into a fingerprint, and use machine learning methods to create a mapping to the vectorial atomic forces.

Only a single pair_coeff command is used with the *agni* style which specifies an AGNI potential file containing the parameters of the force field for the needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of AGNI elements to atom types

See the *pair_coeff* doc page for alternate ways to specify the path for the force field file.

An AGNI force field is fully specified by the filename which contains the parameters of the force field, i.e., the reference training environments used to construct the machine learning force field. Example force field and input files are provided in the examples/USER/misc/agni directory.

Styles with *omp* suffix is functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated style takes the same arguments and should produce the same results, except for round-off and precision issues.

The accelerated style is part of the USER-OMP. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated style explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.4.4 Restrictions

Currently, only elemental systems are implemented. Also, the method only provides access to the forces and not energies or stresses. The lack of potential energy data makes this pair style incompatible with several of the *minimizer algorthms* like *cg* or *sd*. It should work with damped dynamics based minimizers like *fire* or *quickmin*. However, one can access the energy via thermodynamic integration of the forces as discussed in *(Botu3)*. This pair style is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

The AGNI force field files provided with LAMMPS (see the potentials directory) are parameterized for metal *units*. You can use the AGNI potential with any LAMMPS units, but you would need to create your own AGNI potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

18.4.5 Related commands

pair_coeff

Default: none

(Botu1) V. Botu and R. Ramprasad, Int. J. Quant. Chem., 115(16), 1074 (2015).

(Botu2) V. Botu and R. Ramprasad, Phys. Rev. B, 92(9), 094306 (2015).

(Botu3) V. Botu, R. Batra, J. Chapman and R. Ramprasad, https://arxiv.org/abs/1610.02098 (2016).

18.5 pair_style airebo command

18.6 pair_style airebo/intel command

18.7 pair_style airebo/omp command

18.8 pair_style airebo/morse command

18.9 pair_style airebo/morse/intel command

18.10 pair_style airebo/morse/omp command

18.11 pair_style rebo command

18.12 pair_style rebo/intel command

18.13 pair_style rebo/omp command

18.13.1 Syntax

```
pair_style style cutoff LJ_flag TORSION_flag cutoff_min
```

- style = *airebo* or *airebo/morse* or *rebo*
- cutoff = LJ or Morse cutoff (σ scale factor) (AIREBO and AIREBO-M only)
- LJ_flag = 0/1 to turn off/on the LJ or Morse term (AIREBO and AIREBO-M only, optional)
- TORSION_flag = 0/1 to turn off/on the torsion term (AIREBO and AIREBO-M only, optional)
- cutoff_min = Start of the transition region of cutoff (σ scale factor) (AIREBO and AIREBO-M only, optional)

18.13.2 Examples

```
pair_style airebo 3.0
pair_style airebo 2.5 1 0
pair_coeff * * ../potentials/CH.airebo H C

pair_style airebo/morse 3.0
pair_coeff * * ../potentials/CH.airebo-m H C

pair_style rebo
pair_coeff * * ../potentials/CH.rebo H C
```

18.13.3 Description

The *airebo* pair style computes the Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) Potential of *(Stuart)* for a system of carbon and/or hydrogen atoms. Note that this is the initial formulation of AIREBO from 2000, not the later formulation.

The *airebo/morse* pair style computes the AIREBO-M potential, which is equivalent to AIREBO, but replaces the LJ term with a Morse potential. The Morse potentials are parameterized by high-quality quantum chemistry (MP2) calculations and do not diverge as quickly as particle density increases. This allows AIREBO-M to retain accuracy to much higher pressures than AIREBO (up to 40 GPa for Polyethylene). Details for this potential and its parameterization are given in *(O'Conner)*.

The *rebo* pair style computes the Reactive Empirical Bond Order (REBO) Potential of *(Brenner)*. Note that this is the so-called 2nd generation REBO from 2002, not the original REBO from 1990. As discussed below, 2nd generation REBO is closely related to the initial AIREBO; it is just a subset of the potential energy terms with a few slightly different parameters

The AIREBO potential consists of three terms:

$$E = \frac{1}{2} \sum_i \sum_{j \neq i} \left[E_{ij}^{\mathrm{REBO}} + E_{ij}^{\mathrm{LJ}} + \sum_{k \neq i,j} \sum_{l \neq i,j,k} E_{kijl}^{\mathrm{TORSION}} \right]$$

By default, all three terms are included. For the *airebo* style, if the first two optional flag arguments to the pair_style command are included, the LJ and torsional terms can be turned off. Note that both or neither of the flags must be included. If both of the LJ an torsional terms are turned off, it becomes the 2nd-generation REBO potential, with a small caveat on the spline fitting procedure mentioned below. This can be specified directly as pair_style *rebo* with no additional arguments.

The detailed formulas for this potential are given in *(Stuart)*; here we provide only a brief description.

The E^{REBO} term has the same functional form as the hydrocarbon REBO potential developed in *(Brenner)*. The coefficients for E^{REBO} in AIREBO are essentially the same as Brenner's potential, but a few fitted spline values are slightly different. For most cases the E^{REBO} term in AIREBO will produce the same energies, forces and statistical averages as the original REBO potential from which it was derived. The E^{REBO} term in the AIREBO potential gives the model its reactive capabilities and only describes short-ranged C-C, C-H and H-H interactions ($r < 2$ Angstroms). These interactions have strong coordination-dependence through a bond order parameter, which adjusts the attraction between the I,J atoms based on the position of other nearby atoms and thus has 3- and 4-body dependence.

The E^{LJ} term adds longer-ranged interactions ($2 < r <$ cutoff) using a form similar to the standard *Lennard Jones potential*. The E^{LJ} term in AIREBO contains a series of switching functions so that the short-ranged LJ repulsion ($1/r^{12}$) does not interfere with the energetics captured by the E^{REBO} term. The extent of the E^{LJ} interactions is determined by the *cutoff* argument to the pair_style command which is a scale factor. For each type pair (C-C, C-H, H-H) the cutoff is obtained by multiplying the scale factor by the sigma value defined in the potential file for that type pair. In the standard AIREBO potential, $\sigma_{CC} = 3.4$ Angstroms, so with a scale factor of 3.0 (the argument in pair_style), the resulting E^{LJ} cutoff would be 10.2 Angstroms.

By default, the longer-ranged interaction is smoothly switched off between 2.16 and 3.0 σ. By specifying *cutoff_min* in addition to *cutoff*, the switching can be configured to take place between *cutoff_min* and *cutoff*. *cutoff_min* can only be specified if all optional arguments are given.

The E^{TORSION} term is an explicit 4-body potential that describes various dihedral angle preferences in hydrocarbon configurations.

Only a single pair_coeff command is used with the *airebo*, *airebo* or *rebo* style which specifies an AIREBO, REBO, or AIREBO-M potential file with parameters for C and H. Note that as of LAMMPS version 15 May 2019 the *rebo* style in LAMMPS uses its own potential file (CH.rebo). These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of AIREBO elements to atom types

See the *pair_coeff* doc page for alternate ways to specify the path for the potential file.

As an example, if your LAMMPS simulation has 4 atom types and you want the 1st 3 to be C, and the 4th to be H, you would use the following pair_coeff command:

```
pair_coeff * * CH.airebo C C C H
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three C arguments map LAMMPS atom types 1,2,3 to the C element in the AIREBO file. The final H argument maps LAMMPS atom type 4 to the H element in the SW file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *airebo* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

The parameters/coefficients for the AIREBO potentials are listed in the CH.airebo file to agree with the original *(Stuart)* paper. Thus the parameters are specific to this potential and the way it was fit, so modifying the file should be done cautiously.

Similarly the parameters/coefficients for the AIREBO-M potentials are listed in the CH.airebo-m file to agree with the *(O'Connor)* paper. Thus the parameters are specific to this potential and the way it was fit, so modifying the file should be done cautiously. The AIREBO-M Morse potentials were parameterized using a cutoff of 3.0 (σ). Modifying this cutoff may impact simulation accuracy.

This pair style tallies a breakdown of the total AIREBO potential energy into sub-categories, which can be accessed via the *compute pair* command as a vector of values of length 3. The 3 values correspond to the following sub-categories:

1. E_{REBO} = REBO energy
2. E_{LJ} = Lennard-Jones energy
3. E_{TORSION} = Torsion energy

To print these quantities to the log file (with descriptive column headings) the following commands could be included in an input script:

```
compute 0 all pair airebo
variable REBO     equal c_0[1]
variable LJ       equal c_0[2]
variable TORSION  equal c_0[3]
thermo_style custom step temp epair v_REBO v_LJ v_TORSION
```

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support the *pair_modify* mix, shift, table, and tail options.

These pair styles do not write their information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner* , *middle*, *outer* keywords.

18.13.4 Restrictions

These pair styles are part of the MANYBODY package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

These pair potentials require the *newton* setting to be "on" for pair interactions.

The CH.airebo and CH.airebo-m potential files provided with LAMMPS (see the potentials directory) are parameterized for metal *units*. You can use the AIREBO, AIREBO-M or REBO potential with any LAMMPS units, but you would need to create your own AIREBO or AIREBO-M potential file with coefficients listed in the appropriate units, if your simulation doesn't use "metal" units.

18.13.5 Related commands

pair_coeff

Default: none

(Stuart) Stuart, Tutein, Harrison, J Chem Phys, 112, 6472-6486 (2000).

(Brenner) Brenner, Shenderova, Harrison, Stuart, Ni, Sinnott, J Physics: Condensed Matter, 14, 783-802 (2002).

(O'Connor) O'Connor et al., J. Chem. Phys. 142, 024903 (2015).

18.14 pair_style atm command

18.14.1 Syntax

```
pair_style atm cutoff cutoff_triple
```

- cutoff = cutoff for each pair in 3-body interaction (distance units)
- cutoff_triple = additional cutoff applied to product of 3 pairwise distances (distance units)

18.14.2 Examples

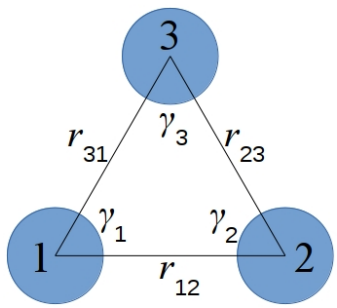
```
pair_style atm 4.5 2.5
pair_coeff * * * 0.072

pair_style hybrid/overlay lj/cut 6.5 atm 4.5 2.5
pair_coeff * * lj/cut 1.0 1.0
pair_coeff 1 1 atm 1 0.064
pair_coeff 1 1 atm 2 0.080
pair_coeff 1 2 atm 2 0.100
pair_coeff 2 2 atm 2 0.125
```

18.14.3 Description

The *atm* style computes a 3-body *Axilrod-Teller-Muto* potential for the energy E of a system of atoms as

$$E = \nu \frac{1 + 3\cos\gamma_1\cos\gamma_2\cos\gamma_3}{r_{12}^3 r_{23}^3 r_{31}^3}$$

where ν is the three-body interaction strength. The distances between pairs of atoms r_{12}, r_{23}, r_{31} and the angles γ_1, γ_2, γ_3 are as shown in this diagram:



Note that for the interaction between a triplet of atoms I, J, K, there is no "central" atom. The interaction is symmetric with respect to permutation of the three atoms. Thus the ν value is the same for all those permutations of the atom types of I, J, K and needs to be specified only once, as discussed below.

The *atm* potential is typically used in combination with a two-body potential using the *pair_style hybrid/overlay* command as in the example above.

The potential for a triplet of atom is calculated only if all 3 distances r_{12}, r_{23}, r_{31} between the 3 atoms satisfy $r_{IJ} <$ cutoff. In addition, the product of the 3 distances $r_{12}r_{23}r_{31}$ < cutoff_triple ^{3} is required, which excludes from calculation the triplets with small contribution to the interaction.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the restart files read by the *read_restart* commands:

- K = atom type of the third atom (1 to N_{types})
- ν = prefactor (energy/distance^9 units)

K can be specified in one of two ways. An explicit numeric value can be used, as in the 2nd example above. $J \leq K$ is required. LAMMPS sets the coefficients for the other 5 symmetric interactions to the same values. E.g. if $I = 1$, $J = 2$, $K = 3$, then these 6 values are set to the specified ν: ν_{123}, ν_{132}, ν_{213}, ν_{231}, ν_{312}, ν_{321}. This enforces the symmetry discussed above.

A wildcard asterisk can be used for K to set the coefficients for multiple triplets of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N equals the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). Note that only type triplets with $J \leq K$ are considered; if asterisks imply type triplets where $K < J$, they are ignored.

Note that a pair_coeff command can override a previous setting for the same I, J, K triplet. For example, these commands set ν for all $I, J.K$ triplets, then overwrite nu for just the $I, J, K = 2, 3, 4$ triplet:

```
pair_coeff * * * 0.25
pair_coeff 2 3 4 0.1
```

Note that for a simulation with a single atom type, only a single entry is required, e.g.

```
pair_coeff 1 1 1 0.25
```

For a simulation with two atom types, four pair_coeff commands will specify all possible nu values:

```
pair_coeff 1 1 1 nu1
pair_coeff 1 1 2 nu2
pair_coeff 1 2 2 nu3
pair_coeff 2 2 2 nu4
```

For a simulation with three atom types, ten pair_coeff commands will specify all possible nu values:

```
pair_coeff 1 1 1 nu1
pair_coeff 1 1 2 nu2
pair_coeff 1 1 3 nu3
pair_coeff 1 2 2 nu4
pair_coeff 1 2 3 nu5
pair_coeff 1 3 3 nu6
pair_coeff 2 2 2 nu7
pair_coeff 2 2 3 nu8
pair_coeff 2 3 3 nu9
pair_coeff 3 3 3 nu10
```

By default the ν value for all triplets is set to 0.0. Thus it is not required to provide pair_coeff commands that enumerate triplet interactions for all K types. If some I, J, K combination is not specified, then there will be no 3-body ATM interactions for that combination and all its permutations. However, as with all pair styles, it is required to specify a pair_coeff command for all I, J combinations, else an error will result.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair styles do not support the *pair_modify* mix, shift, table, and tail options.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file. However, if the *atm* potential is used in combination with other potentials using the *pair_style hybrid/overlay* command then pair_coeff commands need to be re-specified in the restart input script.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner* , *middle* , *outer* keywords.

18.14.4 Restrictions

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.14.5 Related commands

pair_coeff

Default: none

(Axilrod) Axilrod and Teller, J Chem Phys, 11, 299 (1943); Muto, Nippon Sugaku-Buturigakkwaishi 17, 629 (1943).

18.15 pair_style awpmd/cut command

18.15.1 Syntax

```
pair_style awpmd/cut Rc keyword value ...
```

- Rc = global cutoff, -1 means cutoff of half the shortest box length
- zero or more keyword/value pairs may be appended
- keyword = *hartree* or *dproduct* or *uhf* or *free* or *pbc* or *fix* or *harm* or *ermscale* or *flex_press*

```
hartree value = none
dproduct value = none
uhf value = none
free value = none
pbc value = Plen
  Plen = periodic width of electron = -1 or positive value (distance␣
↪units)
fix value = Flen
  Flen = fixed width of electron = -1 or positive value (distance units)
harm value = width
  width = harmonic width constraint
ermscale value = factor
  factor = scaling between electron mass and width variable mass
flex_press value = none
```

18.15.2 Examples

```
pair_style awpmd/cut -1
pair_style awpmd/cut 40.0 uhf free
pair_coeff * *
pair_coeff 2 2 20.0
```

18.15.3 Description

This pair style contains an implementation of the Antisymmetrized Wave Packet Molecular Dynamics (AWPMD) method. Need citation here. Need basic formulas here. Could be links to other documents.

Rc is the cutoff.

The pair_style command allows for several optional keywords to be specified.

The *hartree*, *dproduct*, and *uhf* keywords specify the form of the initial trial wave function for the system. If the *hartree* keyword is used, then a Hartree multielectron trial wave function is used. If the *dproduct* keyword is used, then a trial function which is a product of two determinants for each spin type is used. If the *uhf* keyword is used, then an unrestricted Hartree-Fock trial wave function is used.

The *free*, *pbc*, and *fix* keywords specify a width constraint on the electron wave packets. If the *free* keyword is specified, then there is no constraint. If the *pbc* keyword is used and *Plen* is specified as -1, then the maximum width is half the shortest box length. If *Plen* is a positive value, then the value is the maximum width. If the *fix* keyword is used and *Flen* is specified as -1, then electrons have a constant width that is read from the data file. If *Flen* is a positive value, then the constant width for all electrons is set to *Flen*.

The *harm* keyword allow oscillations in the width of the electron wave packets. More details are needed.

The *ermscale* keyword specifies a unitless scaling factor between the electron masses and the width variable mass. More details needed.

If the *flex_press* keyword is used, then a contribution from the electrons is added to the total virial and pressure of the system.

This potential is designed to be used with *atom_style wavepacket* definitions, in order to handle the description of systems with interacting nuclei and explicit electrons.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- cutoff (distance units)

For *awpmd/cut*, the cutoff coefficient is optional. If it is not used (as in some of the examples above), the default global value specified in the pair_style command is used.

Mixing, shift, table, tail correction, restart, rRESPA info:

The *pair_modify* mix, shift, table, and tail options are not relevant for this pair style.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.15.4 Restrictions

none

18.15.5 Related commands

pair_coeff

18.15.6 Default

These are the defaults for the pair_style keywords: *hartree* for the initial wave function, *free* for the wave packet width.

18.16 pair_style beck command

18.17 pair_style beck/gpu command

18.18 pair_style beck/omp command

18.18.1 Syntax

```
pair_style beck Rc
```

- Rc = cutoff for interactions (distance units)

18.18.2 Examples

```
pair_style beck 8.0
pair_coeff * * 399.671876712 0.0000867636112694 0.675 4.390 0.0003746
pair_coeff 1 1 399.671876712 0.0000867636112694 0.675 4.390 0.0003746 6.0
```

18.18.3 Description

Style *beck* computes interactions based on the potential by *(Beck)*, originally designed for simulation of Helium. It includes truncation at a cutoff distance Rc.

$$E(r) = A \exp\left[-\alpha r - \beta r^6\right] - \frac{B}{\left(r^2+a^2\right)^3}\left(1 + \frac{2.709+3a^2}{r^2+a^2}\right) \qquad r < R_c$$

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands.

- A (energy units)
- B (energy-distance^6 units)
- a (distance units)
- α (1/distance units)
- β (1/distance^6 units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global cutoff R_c is used.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, coefficients must be specified. No default mixing rules are used.

This pair style does not support the *pair_modify* shift option for the energy of the pair interaction.

The *pair_modify* table option is not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.18.4 Restrictions

none

18.18.5 Related commands

pair_coeff

Default: none

(Beck) Beck, Molecular Physics, 14, 311 (1968).

18.19 pair_style body/nparticle command

18.19.1 Syntax

```
pair_style body/nparticle cutoff
```

cutoff = global cutoff for interactions (distance units)

18.19.2 Examples

```
pair_style body/nparticle 3.0
pair_coeff * * 1.0 1.0
pair_coeff 1 1 1.0 1.5 2.5
```

18.19.3 Description

Style *body/nparticle* is for use with body particles and calculates pairwise body/body interactions as well as interactions between body and point-particles. See the *Howto body* doc page for more details on using body particles.

This pair style is designed for use with the "nparticle" body style, which is specified as an argument to the "atom-style body" command. See the *Howto body* doc page for more details about the body styles LAMMPS supports. The "nparticle" style treats a body particle as a rigid body composed of N sub-particles.

The coordinates of a body particle are its center-of-mass (COM). If the COMs of a pair of body particles are within the cutoff (global or type-specific, as specified above), then all interactions between pairs of sub-particles in the two body particles are computed. E.g. if the first body particle has 3 sub-particles, and the second has 10, then 30 interactions are computed and summed to yield the total force and torque on each body particle.

Note: In the example just described, all 30 interactions are computed even if the distance between a particular pair of sub-particles is greater than the cutoff. Likewise, no interaction between two body particles is computed if the two COMs are further apart than the cutoff, even if the distance between some pairs of their sub-particles is within the cutoff. Thus care should be used in defining the cutoff distances for body particles, depending on their shape and size.

Similar rules apply for a body particle interacting with a point particle. The distance between the two particles is calculated using the COM of the body particle and the position of the point particle. If the distance is within the cutoff and the body particle has N sub-particles, then N interactions with the point particle are computed and summed. If the distance is not within the cutoff, no interactions between the body and point particle are computed.

The interaction between two sub-particles, or a sub-particle and point particle, or between two point particles is computed as a Lennard-Jones interaction, using the standard formula

$$E = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \qquad r < R_c$$

where R_c is the cutoff. As explained above, an interaction involving one or two body sub-particles may be computed even for $r > R_c$.

For style *body*, the following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- ϵ (energy units)
- σ (distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global cutoff is used.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of this pair style can be mixed. The default mix value is *geometric*. See the *pair_modify* command for details.

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style does not write its information to *binary restart files*.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.19.4 Restrictions

This style is part of the BODY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Defining particles to be bodies so they participate in body/body or body/particle interactions requires the use of the *atom_style body* command.

18.19.5 Related commands

pair_coeff, *fix rigid*

Default: none

18.20 pair_style body/rounded/polygon command

18.20.1 Syntax

```
pair_style body/rounded/polygon c_n c_t mu delta_ua cutoff
```

```
c_n = normal damping coefficient
c_t = tangential damping coefficient
mu = normal friction coefficient during gross sliding
delta_ua = multiple contact scaling factor
cutoff = global separation cutoff for interactions (distance units), see below for␣
↪definition
```

18.20.2 Examples

```
pair_style body/rounded/polygon 20.0 5.0 0.0 1.0 0.5
pair_coeff * * 100.0 1.0
pair_coeff 1 1 100.0 1.0
```

18.20.3 Description

Style *body/rounded/polygon* is for use with 2d models of body particles of style *rounded/polygon*. It calculates pairwise body/body interactions which can include body particles modeled as 1-vertex circular disks with a specified diameter. See the *Howto body* doc page for more details on using body rounded/polygon particles.

This pairwise interaction between rounded polygons is described in *Fraige*, where a polygon does not have sharp corners, but is rounded at its vertices by circles centered on each vertex with a specified diameter. The edges of the polygon are defined between pairs of adjacent vertices. The circle diameter for each polygon is specified in the data file read by the *read data* command. This is a 2d discrete element model (DEM) which allows for multiple contact points.

Note that when two particles interact, the effective surface of each polygon particle is displaced outward from each of its vertices and edges by half its circle diameter (as in the diagram below of a gray and yellow square particle). The interaction forces and energies between two particles are defined with respect to the separation of their respective rounded surfaces, not by the separation of the vertices and edges themselves.

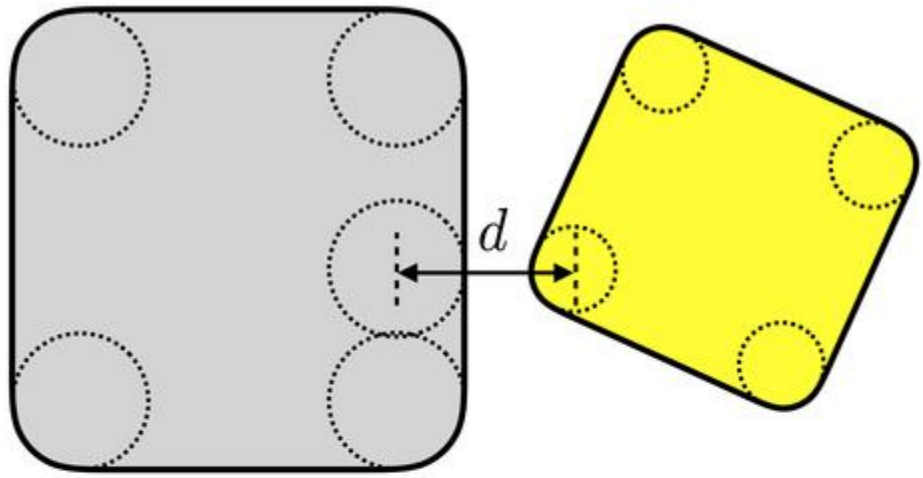
This means that the specified cutoff in the pair_style command is the cutoff distance, r_c, for the surface separation, δ_n (see figure below). This is the distance at which two particles no longer interact. If r_c is specified as 0.0, then it is a contact-only interaction. I.e. the two particles must overlap in order to exert a repulsive force on each other. If $r_c > 0.0$, then the force between two particles will be attractive for surface separations from 0 to r_c, and repulsive once the particles overlap.

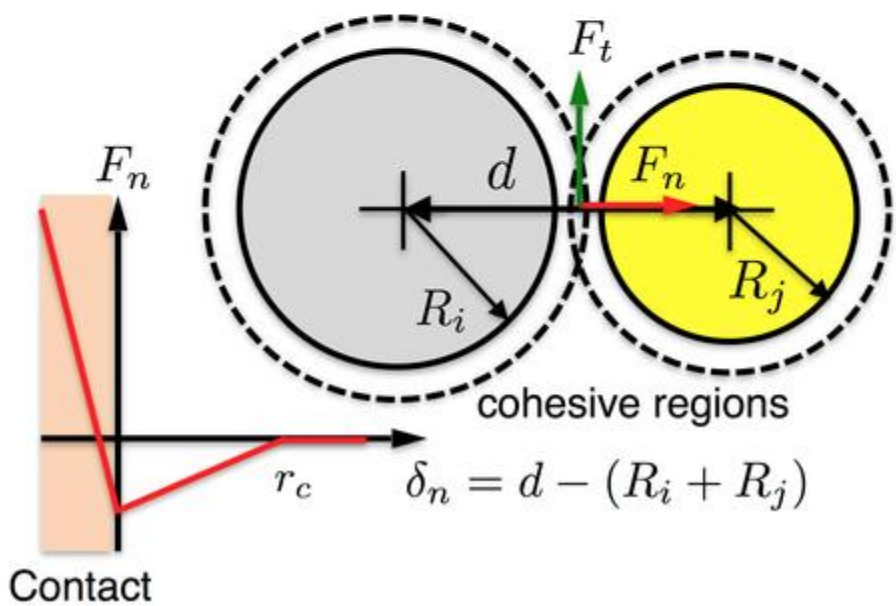
Note that unlike for other pair styles, the specified cutoff is not the distance between the centers of two particles at which they stop interacting. This center-to-center distance depends on the shape and size of the two particles and their relative orientation. LAMMPS takes that into account when computing the surface separation distance and applying the r_c cutoff.

The forces between vertex-vertex, vertex-edge, and edge-edge overlaps are given by:

$$F_n = \begin{cases} k_n\delta_n - c_n v_n & \delta_n \leq 0 \\ -k_{na}\delta_n - c_n v_n & 0 < \delta_n \leq r_c \\ 0 & \delta_n > r_c \end{cases}$$

$$F_t = \begin{cases} \mu k_n \delta_n - c_t v_t & \delta_n \leq 0 \\ 0 & \delta_n > 0 \end{cases}$$





Note that F_n and F_t are functions of the surface separation $\delta_n = d - (R_i + R_j)$. In this model, when $(R_i + R_j) < d < (R_i + R_j) + r_c$, that is, $0 < \delta_n < r_c$, the cohesive region of the two surfaces overlap and the two surfaces are attractive to each other.

In *Fraige*, the tangential friction force between two particles that are in contact is modeled differently prior to gross sliding (i.e. static friction) and during gross-sliding (kinetic friction). The latter takes place when the tangential

deformation exceeds the Coulomb frictional limit. In the current implementation, however, we do not take into account frictional history, i.e. we do not keep track of how many time steps the two particles have been in contact nor calculate the tangential deformation. Instead, we assume that gross sliding takes place as soon as two particles are in contact.

The following coefficients must be defined for each pair of atom types via the *pair_coeff* command as in the examples above, or in the data file read by the *read_data* command:

- k_n (energy/distance^2 units)
- k_{na} (energy/distance^2 units)

Effectively, k_n and k_{na} are the slopes of the red lines in the plot above for force versus surface separation, for $\delta_n < 0$ and $0 < \delta_n < r_c$ respectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the *pair_modify* mix, shift, table, and tail options.

This pair style does not write its information to *binary restart files*. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.20.4 Restrictions

These pair styles are part of the BODY package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This pair style requires the *newton* setting to be "on" for pair interactions.

18.20.5 Related commands

pair_coeff

Default: none

(Fraige) F. Y. Fraige, P. A. Langston, A. J. Matchett, J. Dodds, Particuology, 6, 455 (2008).

18.21 pair_style body/rounded/polyhedron command

18.21.1 Syntax

```
pair_style body/rounded/polyhedron c_n c_t mu delta_ua cutoff
```

```
c_n = normal damping coefficient
c_t = tangential damping coefficient
mu = normal friction coefficient during gross sliding
delta_ua = multiple contact scaling factor
cutoff = global separation cutoff for interactions (distance units), see below for␣
↪definition
```

18.21.2 Examples

```
pair_style body/rounded/polyhedron 20.0 5.0 0.0 1.0 0.5
pair_coeff * * 100.0 1.0
pair_coeff 1 1 100.0 1.0
```

18.21.3 Description

Style *body/rounded/polygon* is for use with 3d models of body particles of style *rounded/polyhedron*. It calculates pairwise body/body interactions which can include body particles modeled as 1-vertex spheres with a specified diameter. See the *Howto body* doc page for more details on using body rounded/polyhedron particles.

This pairwise interaction between the rounded polyhedra is described in *Wang*, where a polyhedron does not have sharp corners and edges, but is rounded at its vertices and edges by spheres centered on each vertex with a specified diameter. The edges if the polyhedron are defined between pairs of adjacent vertices. Its faces are defined by a loop of edges. The sphere diameter for each polygon is specified in the data file read by the *read data* command. This is a discrete element model (DEM) which allows for multiple contact points.

Note that when two particles interact, the effective surface of each polyhedron particle is displaced outward from each of its vertices, edges, and faces by half its sphere diameter. The interaction forces and energies between two particles are defined with respect to the separation of their respective rounded surfaces, not by the separation of the vertices, edges, and faces themselves.

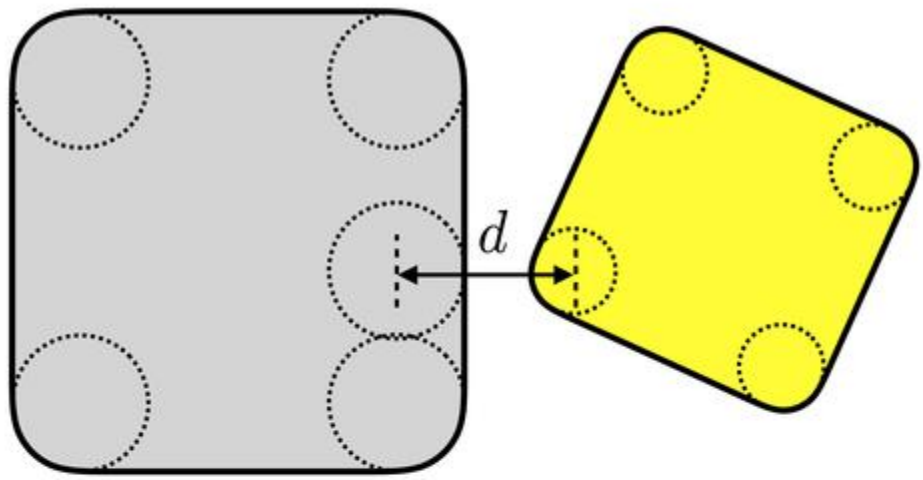
This means that the specified cutoff in the pair_style command is the cutoff distance, r_c, for the surface separation, δ_n (see figure below). This is the distance at which two particles no longer interact. If r_c is specified as 0.0, then it is a contact-only interaction. I.e. the two particles must overlap in order to exert a repulsive force on each other. If $r_c > 0.0$, then the force between two particles will be attractive for surface separations from 0 to r_c, and repulsive once the particles overlap.

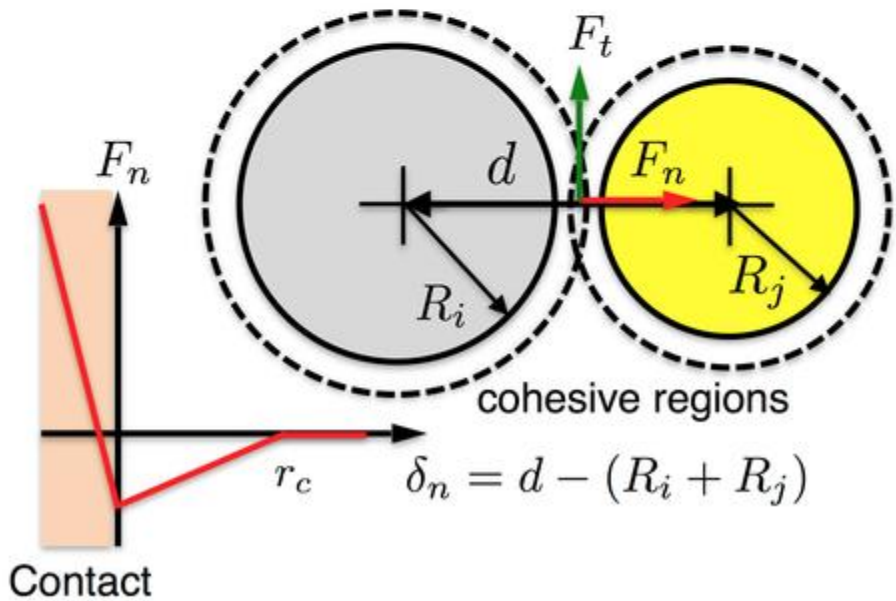
Note that unlike for other pair styles, the specified cutoff is not the distance between the centers of two particles at which they stop interacting. This center-to-center distance depends on the shape and size of the two particles and their relative orientation. LAMMPS takes that into account when computing the surface separation distance and applying the r_c cutoff.

The forces between vertex-vertex, vertex-edge, vertex-face, edge-edge, and edge-face overlaps are given by:

$$F_n = \begin{cases} k_n\delta_n - c_n v_n, & \delta_n \leq 0 \\ -k_{na}\delta_n - c_n v_n & 0 < \delta_n \leq r_c \\ 0 & \delta_n > r_c \end{cases}$$

$$F_t = \begin{cases} \mu k_n \delta_n - c_t v_t & \delta_n \leq 0 \\ 0 & \delta_n > 0 \end{cases}$$





In *Wang*, the tangential friction force between two particles that are in contact is modeled differently prior to gross sliding (i.e. static friction) and during gross-sliding (kinetic friction). The latter takes place when the tangential deformation exceeds the Coulomb frictional limit. In the current implementation, however, we do not take into account frictional history, i.e. we do not keep track of how many time steps the two particles have been in contact nor calculate the tangential deformation. Instead, we assume that gross sliding takes place as soon as two particles are in contact.

The following coefficients must be defined for each pair of atom types via the *pair_coeff* command as in the examples above, or in the data file read by the *read_data* command:

- k_n (energy/distance^2 units)
- k_{na} (energy/distance^2 units)

Effectively, k_n and k_{na} are the slopes of the red lines in the plot above for force versus surface separation, for $\delta_n < 0$ and $0 < \delta_n < r_c$ respectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the *pair_modify* mix, shift, table, and tail options.

This pair style does not write its information to *binary restart files*. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.21.4 Restrictions

These pair styles are part of the BODY package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This pair style requires the *newton* setting to be "on" for pair interactions.

18.21.5 Related commands

pair_coeff

Default: none

(Wang) J. Wang, H. S. Yu, P. A. Langston, F. Y. Fraige, Granular Matter, 13, 1 (2011).

18.22 pair_style bop command

18.22.1 Syntax

```
pair_style bop keyword ...
```

- zero or more keywords may be appended
- keyword = *save*

```
save = pre-compute and save some values
```

18.22.2 Examples

```
pair_style bop
pair_coeff * * ../potentials/CdTe_bop Cd Te
pair_style bop save
pair_coeff * * ../potentials/CdTe.bop.table Cd Te Te
comm_modify cutoff 14.70
```

18.22.3 Description

The *bop* pair style computes Bond-Order Potentials (BOP) based on quantum mechanical theory incorporating both σ and π bonding. By analytically deriving the BOP from quantum mechanical theory its transferability to different phases can approach that of quantum mechanical methods. This potential is similar to the original BOP developed by Pettifor (*Pettifor_1*, *Pettifor_2*, *Pettifor_3*) and later updated by Murdick, Zhou, and Ward (*Murdick*, *Ward*). Currently, BOP potential files for these systems are provided with LAMMPS: AlCu, CCu, CdTe, CdTeSe, CdZnTe, CuH, GaAs. A system with only a subset of these elements, including a single element (e.g. C or Cu or Al or Ga or Zn or CdZn), can also be modeled by using the appropriate alloy file and assigning all atom types to the single element or subset of elements via the pair_coeff command, as discussed below.

The BOP potential consists of three terms:

$$E = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=i_1}^{i_N}\phi_{ij}\left(r_{ij}\right) - \sum_{i=1}^{N}\sum_{j=i_1}^{i_N}\beta_{\sigma,ij}\left(r_{ij}\right)\cdot\Theta_{\sigma,ij} - \sum_{i=1}^{N}\sum_{j=i_1}^{i_N}\beta_{\pi,ij}\left(r_{ij}\right)\cdot\Theta_{\pi,ij} + U_{prom}$$

where $\phi_{ij}(r_{ij})$ is a short-range two-body function representing the repulsion between a pair of ion cores, $\beta_{\sigma,ij}(r_{ij})$ and $\beta_{\sigma,ij}(r_{ij})$ are respectively sigma and π bond integrals, $\Theta_{\sigma,ij}$ and $\Theta_{\pi,ij}$ are σ and π bond-orders, and U_prom is the promotion energy for sp-valent systems.

The detailed formulas for this potential are given in Ward (*Ward*); here we provide only a brief description.

The repulsive energy $\phi_{ij}(r_{ij})$ and the bond integrals $\beta_{\sigma,ij}(r_{ij})$ and $\beta_{\phi,ij}(r_{ij})$ are functions of the interatomic distance r_{ij} between atom *i* and *j*. Each of these potentials has a smooth cutoff at a radius of $r_{cut,ij}$. These smooth cutoffs ensure stable behavior at situations with high sampling near the cutoff such as melts and surfaces.

The bond-orders can be viewed as environment-dependent local variables that are ij bond specific. The maximum value of the σ bond-order (Θ_σ is 1, while that of the π bond-order (Θ_π) is 2, attributing to a maximum value of the total bond-order ($\Theta_\sigma + \Theta_\pi$) of 3. The σ and π bond-orders reflect the ubiquitous single-, double-, and triple- bond behavior of chemistry. Their analytical expressions can be derived from tight- binding theory by recursively expanding an inter-site Green's function as a continued fraction. To accurately represent the bonding with a computationally efficient potential formulation suitable for MD simulations, the derived BOP only takes (and retains) the first two levels of the recursive representations for both the σ and the π bond-orders. Bond-order terms can be understood in terms of molecular orbital hopping paths based upon the Cyrot-Lackmann theorem (*Pettifor_1*). The σ bond-order with a half-full valence shell is used to interpolate the bond-order expression that incorporated explicit valance band filling. This π bond-order expression also contains also contains a three-member ring term that allows implementation of an asymmetric density of states, which helps to either stabilize or destabilize close-packed structures. The π bond-order includes hopping paths of length 4. This enables the incorporation of dihedral angles effects.

Note: Note that unlike for other potentials, cutoffs for BOP potentials are not set in the pair_style or pair_coeff command; they are specified in the BOP potential files themselves. Likewise, the BOP potential files list atomic masses; thus you do not need to use the *mass* command to specify them. Note that for BOP potentials with hydrogen, you will likely want to set the mass of H atoms to be 10x or 20x larger to avoid having to use a tiny timestep. You can do this by using the *mass* command after using the *pair_coeff* command to read the BOP potential file.

One option can be specified as a keyword with the pair_style command.

The *save* keyword gives you the option to calculate in advance and store a set of distances, angles, and derivatives of angles. The default is to not do this, but to calculate them on-the-fly each time they are needed. The former may be faster, but takes more memory. The latter requires less memory, but may be slower. It is best to test this option to optimize the speed of BOP for your particular system configuration.

Only a single pair_coeff command is used with the *bop* style which specifies a BOP potential file, with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of BOP elements to atom types

As an example, imagine the CdTe.bop file has BOP values for Cd and Te. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Cd, and the 4th to be Te, you would use the following pair_coeff command:

```
pair_coeff * * CdTe Cd Cd Cd Te
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Cd arguments map LAMMPS atom types 1,2,3 to the Cd element in the BOP file. The final Te argument maps LAMMPS atom type 4 to the Te element in the BOP file.

BOP files in the *potentials* directory of the LAMMPS distribution have a ".bop" suffix. The potentials are in tabulated form containing pre-tabulated pair functions for phi_ij(r_ij), beta_(sigma,ij)(r_ij), and beta_pi,ij)(r_ij).

The parameters/coefficients format for the different kinds of BOP files are given below with variables matching the formulation of Ward (*Ward*) and Zhou (*Zhou*). Each header line containing a ":" is preceded by a blank line.

No angular table file format:

The parameters/coefficients format for the BOP potentials input file containing pre-tabulated functions of g is given below with variables matching the formulation of Ward (*Ward*). This format also assumes the angular functions have the formulation of (*Ward*).

- Line 1: # elements N

The first line is followed by N lines containing the atomic number, mass, and element symbol of each element.

Following the definition of the elements several global variables for the tabulated functions are given.

- Line 1: nr, nBOt (nr is the number of divisions the radius is broken into for function tables and MUST be a factor of 5; nBOt is the number of divisions for the tabulated values of THETA_(S,ij)
- Line 2: delta_1-delta_7 (if all are not used in the particular
- formulation, set unused values to 0.0)

Following this N lines for e_1-e_N containing p_pi.

- Line 3: p_pi (for e_1)
- Line 4: p_pi (for e_2 and continues to e_N)

The next section contains several pair constants for the number of interaction types e_i-e_j, with i=1->N, j=i->N

- Line 1: r_cut (for e_1-e_1 interactions)
- Line 2: c_sigma, a_sigma, c_pi, a_pi
- Line 3: delta_sigma, delta_pi
- Line 4: f_sigma, k_sigma, delta_3 (This delta_3 is similar to that of the previous section but is interaction type dependent)

The next section contains a line for each three body interaction type e_j-e_i-e_k with i=0->N, j=0->N, k=j->N

- Line 1: g_(sigma0), g_(sigma1), g_(sigma2) (These are coefficients for g_(sigma,jik)(THETA_ijk) for e_1-e_1-e_1 interaction. *Ward* contains the full expressions for the constants as functions of b_(sigma,ijk), p_(sigma,ijk), u_(sigma,ijk))
- Line 2: g_(sigma0), g_(sigma1), g_(sigma2) (for e_1-e_1-e_2)

The next section contains a block for each interaction type for the phi_ij(r_ij). Each block has nr entries with 5 entries per line.

- Line 1: phi(r1), phi(r2), phi(r3), phi(r4), phi(r5) (for the e_1-e_1 interaction type)
- Line 2: phi(r6), phi(r7), phi(r8), phi(r9), phi(r10) (this continues until nr)
- ...
- Line nr/5_1: phi(r1), phi(r2), phi(r3), phi(r4), phi(r5), (for the e_1-e_1 interaction type)

The next section contains a block for each interaction type for the beta_(sigma,ij)(r_ij). Each block has nr entries with 5 entries per line.

- Line 1: beta_sigma(r1), beta_sigma(r2), beta_sigma(r3), beta_sigma(r4), beta_sigma(r5) (for the e_1-e_1 interaction type)
- Line 2: beta_sigma(r6), beta_sigma(r7), beta_sigma(r8), beta_sigma(r9), beta_sigma(r10) (this continues until nr)
- ...
- Line nr/5+1: beta_sigma(r1), beta_sigma(r2), beta_sigma(r3), beta_sigma(r4), beta_sigma(r5) (for the e_1-e_2 interaction type)

The next section contains a block for each interaction type for beta_(pi,ij)(r_ij). Each block has nr entries with 5 entries per line.

- Line 1: beta_pi(r1), beta_pi(r2), beta_pi(r3), beta_pi(r4), beta_pi(r5) (for the e_1-e_1 interaction type)
- Line 2: beta_pi(r6), beta_pi(r7), beta_pi(r8), beta_pi(r9), beta_pi(r10) (this continues until nr)
- ...
- Line nr/5+1: beta_pi(r1), beta_pi(r2), beta_pi(r3), beta_pi(r4), beta_pi(r5) (for the e_1-e_2 interaction type)

The next section contains a block for each interaction type for the THETA_(S,ij)((THETA_(sigma,ij))^(1/2), f_(sigma,ij)). Each block has nBOt entries with 5 entries per line.

- Line 1: THETA_(S,ij)(r1), THETA_(S,ij)(r2), THETA_(S,ij)(r3), THETA_(S,ij)(r4), THETA_(S,ij)(r5) (for the e_1-e_2 interaction type)
- Line 2: THETA_(S,ij)(r6), THETA_(S,ij)(r7), THETA_(S,ij)(r8), THETA_(S,ij)(r9), THETA_(S,ij)(r10) (this continues until nBOt)
- ...
- Line nBOt/5+1: THETA_(S,ij)(r1), THETA_(S,ij)(r2), THETA_(S,ij)(r3), THETA_(S,ij)(r4), THETA_(S,ij)(r5) (for the e_1-e_2 interaction type)

The next section contains a block of N lines for e_1-e_N

- Line 1: delta^mu (for e_1)
- Line 2: delta^mu (for e_2 and repeats to e_N)

The last section contains more constants for e_i-e_j interactions with i=0->N, j=i->N

- Line 1: (A_ij)^(mu*nu) (for e1-e1)
- Line 2: (A_ij)^(mu*nu) (for e1-e2 and repeats as above)

Angular spline table file format:

The parameters/coefficients format for the BOP potentials input file containing pre-tabulated functions of g is given below with variables matching the formulation of Ward (*Ward*). This format also assumes the angular functions have the formulation of (*Zhou*).

- Line 1: # elements N

The first line is followed by N lines containing the atomic number, mass, and element symbol of each element.

Following the definition of the elements several global variables for the tabulated functions are given.

- Line 1: nr, ntheta, nBOt (nr is the number of divisions the radius is broken into for function tables and MUST be a factor of 5; ntheta is the power of the power of the spline used to fit the angular function; nBOt is the number of divisions for the tabulated values of THETA_(S,ij)
- Line 2: delta_1-delta_7 (if all are not used in the particular
- formulation, set unused values to 0.0)

Following this N lines for e_1-e_N containing p_pi.

- Line 3: p_pi (for e_1)
- Line 4: p_pi (for e_2 and continues to e_N)

The next section contains several pair constants for the number of interaction types e_i-e_j, with i=1->N, j=i->N

- Line 1: r_cut (for e_1-e_1 interactions)
- Line 2: c_sigma, a_sigma, c_pi, a_pi
- Line 3: delta_sigma, delta_pi
- Line 4: f_sigma, k_sigma, delta_3 (This delta_3 is similar to that of the previous section but is interaction type dependent)

The next section contains a line for each three body interaction type e_j-e_i-e_k with i=0->N, j=0->N, k=j->N

- Line 1: g0, g1, g2… (These are coefficients for the angular spline of the g_(sigma,jik)(THETA_ijk) for e_1-e_1-e_1 interaction. The function can contain up to 10 term thus 10 constants. The first line can contain up to five constants. If the spline has more than five terms the second line will contain the remaining constants The following lines will then contain the constants for the remaining g0, g1, g2… (for e_1-e_1-e_2) and the other three body interactions

The rest of the table has the same structure as the previous section (see above).

Angular no-spline table file format:

The parameters/coefficients format for the BOP potentials input file containing pre-tabulated functions of g is given below with variables matching the formulation of Ward (*Ward*). This format also assumes the angular functions have the formulation of (*Zhou*).

- Line 1: # elements N

The first two lines are followed by N lines containing the atomic number, mass, and element symbol of each element.

Following the definition of the elements several global variables for the tabulated functions are given.

- Line 1: nr, ntheta, nBOt (nr is the number of divisions the radius is broken into for function tables and MUST be a factor of 5; ntheta is the number of divisions for the tabulated values of the g angular function; nBOt is the number of divisions for the tabulated values of THETA_(S,ij)
- Line 2: delta_1-delta_7 (if all are not used in the particular
- formulation, set unused values to 0.0)

Following this N lines for e_1-e_N containing p_pi.

- Line 3: p_pi (for e_1)
- Line 4: p_pi (for e_2 and continues to e_N)

The next section contains several pair constants for the number of interaction types e_i-e_j, with i=1->N, j=i->N

- Line 1: r_cut (for e_1-e_1 interactions)
- Line 2: c_sigma, a_sigma, c_pi, a_pi
- Line 3: delta_sigma, delta_pi
- Line 4: f_sigma, k_sigma, delta_3 (This delta_3 is similar to that of the previous section but is interaction type dependent)

The next section contains a line for each three body interaction type e_j-e_i-e_k with i=0->N, j=0->N, k=j->N

- Line 1: g(theta1), g(theta2), g(theta3), g(theta4), g(theta5) (for the e_1-e_1-e_1 interaction type)
- Line 2: g(theta6), g(theta7), g(theta8), g(theta9), g(theta10) (this continues until ntheta)
- ...
- Line ntheta/5+1: g(theta1), g(theta2), g(theta3), g(theta4), g(theta5), (for the e_1-e_1-e_2 interaction type)

The rest of the table has the same structure as the previous section (see above).

Mixing, shift, table tail correction, restart:

This pair style does not support the *pair_modify* mix, shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.22.4 Restrictions

These pair styles are part of the MANYBODY package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

These pair potentials require the *newton* setting to be "on" for pair interactions.

The CdTe.bop and GaAs.bop potential files provided with LAMMPS (see the potentials directory) are parameterized for metal *units*. You can use the BOP potential with any LAMMPS units, but you would need to create your own BOP potential file with coefficients listed in the appropriate units if your simulation does not use "metal" units.

18.22.5 Related commands

pair_coeff

18.22.6 Default

non-tabulated potential file, a_0 is non-zero.

(Pettifor_1) D.G. Pettifor and I.I. Oleinik, Phys. Rev. B, 59, 8487 (1999).

(Pettifor_2) D.G. Pettifor and I.I. Oleinik, Phys. Rev. Lett., 84, 4124 (2000).

(Pettifor_3) D.G. Pettifor and I.I. Oleinik, Phys. Rev. B, 65, 172103 (2002).

(Murdick) D.A. Murdick, X.W. Zhou, H.N.G. Wadley, D. Nguyen-Manh, R. Drautz, and D.G. Pettifor, Phys. Rev. B, 73, 45206 (2006).

(Ward) D.K. Ward, X.W. Zhou, B.M. Wong, F.P. Doty, and J.A. Zimmerman, Phys. Rev. B, 85,115206 (2012).

(Zhou) X.W. Zhou, D.K. Ward, M. Foster (TBP).

18.23 pair_style born command

18.24 pair_style born/omp command

18.25 pair_style born/gpu command

18.26 pair_style born/coul/long command

18.27 pair_style born/coul/long/gpu command

18.28 pair_style born/coul/long/omp command

18.29 pair_style born/coul/msm command

18.30 pair_style born/coul/msm/omp command

18.31 pair_style born/coul/wolf command

18.32 pair_style born/coul/wolf/gpu command

18.33 pair_style born/coul/wolf/omp command

18.34 pair_style born/coul/dsf command

18.34.1 Syntax

```
pair_style style args
```

- style = *born* or *born/coul/long* or *born/coul/msm* or *born/coul/wolf*
- args = list of arguments for a particular style

```
born args = cutoff
  cutoff = global cutoff for non-Coulombic interactions (distance units)
born/coul/long args = cutoff (cutoff2)
  cutoff = global cutoff for non-Coulombic (and Coulombic if only 1 arg)␣
↪(distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
```

```
born/coul/msm args = cutoff (cutoff2)
  cutoff = global cutoff for non-Coulombic (and Coulombic if only 1 arg)␣
↪(distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
born/coul/wolf args = alpha cutoff (cutoff2)
  alpha = damping parameter (inverse distance units)
  cutoff = global cutoff for non-Coulombic (and Coulombic if only 1 arg)␣
↪(distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
born/coul/dsf args = alpha cutoff (cutoff2)
  alpha = damping parameter (inverse distance units)
  cutoff = global cutoff for non-Coulombic (and Coulombic if only 1 arg)␣
↪(distance units)
  cutoff2 = global cutoff for Coulombic (distance units)
```

18.34.2 Examples

```
pair_style born 10.0
pair_coeff * * 6.08 0.317 2.340 24.18 11.51
pair_coeff 1 1 6.08 0.317 2.340 24.18 11.51

pair_style born/coul/long 10.0
pair_style born/coul/long 10.0 8.
pair_coeff * * 6.08 0.317 2.340 24.18 11.51
pair_coeff 1 1 6.08 0.317 2.340 24.18 11.51

pair_style born/coul/msm 10.0
pair_style born/coul/msm 10.0 8.0
pair_coeff * * 6.08 0.317 2.340 24.18 11.51
pair_coeff 1 1 6.08 0.317 2.340 24.18 11.51

pair_style born/coul/wolf 0.25 10.0
pair_style born/coul/wolf 0.25 10.0 9.0
pair_coeff * * 6.08 0.317 2.340 24.18 11.51
pair_coeff 1 1 6.08 0.317 2.340 24.18 11.51

pair_style born/coul/dsf 0.1 10.0 12.0
pair_coeff * *   0.0 1.00 0.00 0.00 0.00
pair_coeff 1 1 480.0 0.25 0.00 1.05 0.50
```

18.34.3 Description

The *born* style computes the Born-Mayer-Huggins or Tosi/Fumi potential described in *(Fumi and Tosi)*, given by

$$E = A \exp\left(\frac{\sigma - r}{\rho}\right) - \frac{C}{r^6} + \frac{D}{r^8} \qquad r < r_c$$

where σ is an interaction-dependent length parameter, ρ is an ionic-pair dependent length parameter, and r_c is the cutoff.

The styles with *coul/long* or *coul/msm* add a Coulombic term as described for the *lj/cut* pair styles. An additional damping factor is applied to the Coulombic term so it can be used in conjunction with the *kspace_style* command and its *ewald* or *pppm* of *msm* option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

If one cutoff is specified for the *born/coul/long* and *born/coul/msm* style, it is used for both the A,C,D and Coulombic terms. If two cutoffs are specified, the first is used as the cutoff for the A,C,D terms, and the second is the cutoff for the Coulombic term.

The *born/coul/wolf* style adds a Coulombic term as described for the Wolf potential in the *coul/wolf* pair style.

The *born/coul/dsf* style computes the Coulomb contribution with the damped shifted force model as in the *coul/dsf* style.

Note that these potentials are related to the *Buckingham potential*.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- A (energy units)
- ρ (distance units)
- σ (distance units)
- C (energy units * distance units^6)
- D (energy units * distance units^8)
- cutoff (distance units)

The second coefficient, rho, must be greater than zero.

The last coefficient is optional. If not specified, the global A,C,D cutoff specified in the pair_style command is used.

For *born/coul/long*, *born/coul/wolf* and *born/coul/dsf* no Coulombic cutoff can be specified for an individual I,J type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

These styles support the *pair_modify* shift option for the energy of the exp(), 1/r^6, and 1/r^8 portion of the pair interaction.

The *born/coul/long* pair style supports the *pair_modify* table option to tabulate the short-range portion of the long-range Coulombic interaction.

These styles support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

Thess styles writes thei information to binary *restart* files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These styles can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

18.34.4 Restrictions

The *born/coul/long* style is part of the KSPACE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.34.5 Related commands

pair_coeff, *pair_style buck*

Default: none

Fumi and Tosi, J Phys Chem Solids, 25, 31 (1964), Fumi and Tosi, J Phys Chem Solids, 25, 45 (1964).

18.35 pair_style brownian command

18.36 pair_style brownian/omp command

18.37 pair_style brownian/poly command

18.38 pair_style brownian/poly/omp command

18.38.1 Syntax

```
pair_style style mu flaglog flagfld cutinner cutoff t_target seed flagHI flagVF
```

- style = *brownian* or *brownian/poly*
- mu = dynamic viscosity (dynamic viscosity units)
- flaglog = 0/1 log terms in the lubrication approximation on/off
- flagfld = 0/1 to include/exclude Fast Lubrication Dynamics effects
- cutinner = inner cutoff distance (distance units)
- cutoff = outer cutoff for interactions (distance units)
- t_target = target temp of the system (temperature units)
- seed = seed for the random number generator (positive integer)
- flagHI (optional) = 0/1 to include/exclude 1/r hydrodynamic interactions
- flagVF (optional) = 0/1 to include/exclude volume fraction corrections in the long-range isotropic terms

18.38.2 Examples

```
pair_style brownian 1.5 1 1 2.01 2.5 2.0 5878567 (assuming radius = 1)
pair_coeff 1 1 2.05 2.8
pair_coeff * *
```

18.38.3 Description

Styles *brownian* and *brownian/poly* compute Brownian forces and torques on finite-size spherical particles. The former requires monodisperse spherical particles; the latter allows for polydisperse spherical particles.

These pair styles are designed to be used with either the *pair_style lubricate* or *pair_style lubricateU* commands to provide thermostatting when dissipative lubrication forces are acting. Thus the parameters *mu*, *flaglog*, *flagfld*, *cutinner*, and *cutoff* should be specified consistent with the settings in the lubrication pair styles. For details, refer to either of the lubrication pair styles.

The *t_target* setting is used to specify the target temperature of the system. The random number *seed* is used to generate random numbers for the thermostatting procedure.

The *flagHI* and *flagVF* settings are optional. Neither should be used, or both must be defined.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- cutinner (distance units)
- cutoff (distance units)

The two coefficients are optional. If neither is specified, the two cutoffs specified in the pair_style command are used. Otherwise both must be specified.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in *this section* of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See *this section* of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the two cutoff distances for this pair style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style does not support the *pair_modify* shift option for the energy of the pair interaction.

The *pair_modify* table option is not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.38.4 Restrictions

These styles are part of the COLLOID package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Only spherical monodisperse particles are allowed for pair_style brownian.

Only spherical particles are allowed for pair_style brownian/poly.

18.38.5 Related commands

pair_coeff, *pair_style lubricate*, *pair_style lubricateU*

18.38.6 Default

The default settings for the optional args are flagHI = 1 and flagVF = 1.

18.39 pair_style buck command

18.40 pair_style buck/gpu command

18.41 pair_style buck/intel command

18.42 pair_style buck/kk command

18.43 pair_style buck/omp command

18.44 pair_style buck/coul/cut command

18.45 pair_style buck/coul/cut/gpu command

18.46 pair_style buck/coul/cut/intel command

18.47 pair_style buck/coul/cut/kk command

18.48 pair_style buck/coul/cut/omp command

18.49 pair_style buck/coul/long command

18.50 pair_style buck/coul/long/gpu command

18.51 pair_style buck/coul/long/intel command

18.52 pair_style buck/coul/long/kk command

18.53 pair_style buck/coul/long/omp command

18.54 pair_style buck/coul/msm command

18.55 pair_style buck/coul/msm/omp command

18.55.1 Syntax

```
pair_style style args
```

- style = *buck* or *buck/coul/cut* or *buck/coul/long* or *buck/coul/msm*

- args = list of arguments for a particular style

```
buck args = cutoff
  cutoff = global cutoff for Buckingham interactions (distance units)
buck/coul/cut args = cutoff (cutoff2)
  cutoff = global cutoff for Buckingham (and Coulombic if only 1 arg)␣
↪(distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
buck/coul/long args = cutoff (cutoff2)
  cutoff = global cutoff for Buckingham (and Coulombic if only 1 arg)␣
↪(distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
buck/coul/msm args = cutoff (cutoff2)
  cutoff = global cutoff for Buckingham (and Coulombic if only 1 arg)␣
↪(distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
```

18.55.2 Examples

```
pair_style buck 2.5
pair_coeff * * 100.0 1.5 200.0
pair_coeff * * 100.0 1.5 200.0 3.0

pair_style buck/coul/cut 10.0
pair_style buck/coul/cut 10.0 8.0
pair_coeff * * 100.0 1.5 200.0
pair_coeff 1 1 100.0 1.5 200.0 9.0
pair_coeff 1 1 100.0 1.5 200.0 9.0 8.0

pair_style buck/coul/long 10.0
pair_style buck/coul/long 10.0 8.0
pair_coeff * * 100.0 1.5 200.0
pair_coeff 1 1 100.0 1.5 200.0 9.0

pair_style buck/coul/msm 10.0
pair_style buck/coul/msm 10.0 8.0
pair_coeff * * 100.0 1.5 200.0
pair_coeff 1 1 100.0 1.5 200.0 9.0
```

18.55.3 Description

The *buck* style computes a Buckingham potential (exp/6 instead of Lennard-Jones 12/6) given by

$$E = Ae^{-r/\rho} - \frac{C}{r^6} \qquad r < r_c$$

where ρ is an ionic-pair dependent length parameter, and r_c is the cutoff on both terms.

The styles with *coul/cut* or *coul/long* or *coul/msm* add a Coulombic term as described for the *lj/cut* pair styles. For *buck/coul/long* and *buc/coul/msm*, an additional damping factor is applied to the Coulombic term so it can be used in conjunction with the *kspace_style* command and its *ewald* or *pppm* or *msm* option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

If one cutoff is specified for the *born/coul/cut* and *born/coul/long* and *born/coul/msm* styles, it is used for both the A,C and Coulombic terms. If two cutoffs are specified, the first is used as the cutoff for the A,C terms, and the second is the cutoff for the Coulombic term.

Note that these potentials are related to the *Born-Mayer-Huggins potential*.

Note: For all these pair styles, the terms with A and C are always cutoff. The additional Coulombic term can be cutoff or long-range (no cutoff) depending on whether the style name includes coul/cut or coul/long or coul/msm. If you wish the C/r^6 term to be long-range (no cutoff), then see the *pair_style buck/long/coul/long* command.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- A (energy units)
- ρ (distance units)
- C (energy-distance^6 units)
- cutoff (distance units)
- cutoff2 (distance units)

The second coefficient, ρ, must be greater than zero. The coefficients A,:math:*rho*, and C can be written as analytical expressions of ϵ and σ, in analogy to the Lennard-Jones potential *(Khrapak)*.

The latter 2 coefficients are optional. If not specified, the global A,C and Coulombic cutoffs are used. If only one cutoff is specified, it is used as the cutoff for both A,C and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the A,C and Coulombic cutoffs for this type pair. You cannot specify 2 cutoffs for style *buck*, since it has no Coulombic terms. For *buck/coul/long* only the LJ cutoff can be specified since a Coulombic cutoff cannot be specified for an individual I,J type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

These styles support the *pair_modify* shift option for the energy of the exp() and 1/r^6 portion of the pair interaction.

The *buck/coul/long* pair style supports the *pair_modify* table option to tabulate the short-range portion of the long-range Coulombic interaction.

These styles support the pair_modify tail option for adding long-range tail corrections to energy and pressure for the A,C terms in the pair interaction.

These styles write their information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These styles can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

18.55.4 Restrictions

The *buck/coul/long* style is part of the KSPACE package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.55.5 Related commands

pair_coeff, *pair_style born*

Default: none

(Khrapak) Khrapak, Chaudhuri, and Morfill, J Chem Phys, 134, 054120 (2011).

18.56 pair_style buck6d/coul/gauss/dsf command

18.57 pair_style buck6d/coul/gauss/long command

18.57.1 Syntax

```
pair_style style args
```

- style = *buck6d/coul/gauss/dsf* or *buck6d/coul/gauss/long*
- args = list of arguments for a particular style

```
buck6d/coul/gauss/dsf args = smooth cutoff (cutoff2)
  smooth  = smoothing onset within Buckingham cutoff (ratio)
  cutoff  = global cutoff for Buckingham (and Coulombic if only 1 arg)␣
↪(distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
buck6d/coul/gauss/long args = smooth smooth2 cutoff (cutoff2)
  smooth   = smoothing onset within Buckingham cutoff (ratio)
  smooth2  = smoothing onset within Coulombic cutoff (ratio)
  cutoff   = global cutoff for Buckingham (and Coulombic if only 1 arg)␣
↪(distance units)
  cutoff2  = global cutoff for Coulombic (optional) (distance units)
```

18.57.2 Examples

```
pair_style buck6d/coul/gauss/dsf    0.9000    12.0000
pair_coeff 1  1  1030.  3.061  457.179  4.521  0.608

pair_style buck6d/coul/gauss/long   0.9000  1.0000  12.0000
pair_coeff 1  1  1030.  3.061  457.179  4.521  0.608
```

18.57.3 Description

The *buck6d/coul/gauss* styles evaluate vdW and Coulomb interactions following the MOF-FF force field after *(Schmid)*. The vdW term of the *buck6d* styles computes a dispersion damped Buckingham potential:

$$E = Ae^{-\kappa r} - \frac{C}{r^6} \cdot \frac{1}{1 + Dr^{14}} \qquad r < r_c$$

where A and C are a force constant, κ is an ionic-pair dependent reciprocal length parameter, D is a dispersion correction parameter, and the cutoff r_c truncates the interaction distance. The first term in the potential corresponds to the Buckingham repulsion term and the second term to the dispersion attraction with a damping correction analog to the Grimme correction used in DFT. The latter corrects for artifacts occurring at short distances which become an issue for soft vdW potentials.

The *buck6d* styles include a smoothing function which is invoked according to the global smoothing parameter within the specified cutoff. Hereby a parameter of i.e. 0.9 invokes the smoothing within 90% of the cutoff. No smoothing is applied at a value of 1.0. For the *gauss/dsf* style this smoothing is only applicable for the dispersion damped Buckingham potential. For the *gauss/long* styles the smoothing function can also be invoked for the real space coulomb interactions which enforce continuous energies and forces at the cutoff.

Both styles *buck6d/coul/gauss/dsf* and *buck6d/coul/gauss/long* evaluate a Coulomb potential using spherical Gaussian type charge distributions which effectively dampen electrostatic interactions for high charges at close distances. The electrostatic potential is thus evaluated as:

$$E = \frac{C_{q_i q_j}}{\epsilon r_{ij}} \operatorname{erf}(\alpha_{ij} r_{ij}) \qquad r < r_c$$

where C is an energy-conversion constant, q_i and q_j are the charges on the 2 atoms, epsilon is the dielectric constant which can be set by the *dielectric* command, α is the ion pair dependent damping parameter and erf() is the error-function. The cutoff r_c truncates the interaction distance.

The style *buck6d/coul/gauss/dsf* computes the Coulomb interaction via the damped shifted force model described in *(Fennell)* approximating an Ewald sum similar to the *pair coul/dsf* styles. In *buck6d/coul/gauss/long* an additional damping factor is applied to the Coulombic term so it can be used in conjunction with the *kspace_style* command and its *ewald* or *pppm* options. The Coulombic cutoff in this case separates the real and reciprocal space evaluation of the Ewald sum.

If one cutoff is specified it is used for both the vdW and Coulomb terms. If two cutoffs are specified, the first is used as the cutoff for the vdW terms, and the second is the cutoff for the Coulombic term.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- A (energy units)
- ρ (distance^-1 units)
- C (energy-distance^6 units)
- D (distance^14 units)

- α (distance^-1 units)
- cutoff (distance units)

The second coefficient, ρ, must be greater than zero. The latter coefficient is optional. If not specified, the global vdW cutoff is used.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

These styles do not support the *pair_modify* shift option for the energy. Instead the smoothing function should be applied by setting the global smoothing parameter to a value < 1.0.

These styles write their information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

18.57.4 Restrictions

These styles are part of the USER-MOFFF package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.57.5 Related commands

pair_coeff

Default: none

(Schmid) S. Bureekaew, S. Amirjalayer, M. Tafipolsky, C. Spickermann, T.K. Roy and R. Schmid, Phys. Status Solidi B, 6, 1128 (2013).

(Fennell) C. J. Fennell, J. D. Gezelter, J Chem Phys, 124, 234104 (2006).

18.58 pair_style buck/long/coul/long command

18.59 pair_style buck/long/coul/long/omp command

18.59.1 Syntax

```
pair_style buck/long/coul/long flag_buck flag_coul cutoff (cutoff2)
```

- flag_buck = *long* or *cut*

  ```
  long = use Kspace long-range summation for the dispersion term 1/r^6
  cut = use a cutoff
  ```

- flag_coul = *long* or *off*

  ```
  long = use Kspace long-range summation for the Coulombic term 1/r
  off = omit the Coulombic term
  ```

- cutoff = global cutoff for Buckingham (and Coulombic if only 1 cutoff) (distance units)
- cutoff2 = global cutoff for Coulombic (optional) (distance units)

18.59.2 Examples

```
pair_style buck/long/coul/long cut off 2.5
pair_style buck/long/coul/long cut long 2.5 4.0
pair_style buck/long/coul/long long long 4.0
pair_coeff * * 1 1
pair_coeff 1 1 1 3 4
```

18.59.3 Description

The *buck/long/coul/long* style computes a Buckingham potential (exp/6 instead of Lennard-Jones 12/6) and Coulombic potential, given by

$$E = Ae^{-r/\rho} - \frac{C}{r^6} \qquad r < r_c$$
$$E = \frac{Cq_iq_j}{\epsilon r} \qquad r < r_c$$

r_c is the cutoff. If one cutoff is specified in the pair_style command, it is used for both the Buckingham and Coulombic terms. If two cutoffs are specified, they are used as cutoffs for the Buckingham and Coulombic terms respectively.

The purpose of this pair style is to capture long-range interactions resulting from both attractive 1/r^6 Buckingham and Coulombic 1/r interactions. This is done by use of the *flag_buck* and *flag_coul* settings. The *Ismail* paper has more details on when it is appropriate to include long-range 1/r^6 interactions, using this potential.

If *flag_buck* is set to *long*, no cutoff is used on the Buckingham 1/r^6 dispersion term. The long-range portion can be calculated by using the *kspace_style ewald/disp or pppm/disp* commands. The specified Buckingham cutoff then determines which portion of the Buckingham interactions are computed directly by the pair potential versus which part is computed in reciprocal space via the Kspace style. If *flag_buck* is set to *cut*, the Buckingham interactions are simply cutoff, as with *pair_style buck*.

If *flag_coul* is set to *long*, no cutoff is used on the Coulombic interactions. The long-range portion can calculated by using any of several *kspace_style* command options such as *pppm* or *ewald*. Note that if *flag_buck* is also set to long, then the *ewald/disp* or *pppm/disp* Kspace style needs to be used to perform the long-range calculations for both the Buckingham and Coulombic interactions. If *flag_coul* is set to *off*, Coulombic interactions are not computed.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- A (energy units)
- rho (distance units)
- C (energy-distance^6 units)
- cutoff (distance units)
- cutoff2 (distance units)

The second coefficient, rho, must be greater than zero.

The latter 2 coefficients are optional. If not specified, the global Buckingham and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both Buckingham and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the Buckingham and Coulombic cutoffs for this type pair. Note that if you are using *flag_buck* set to *long*, you cannot specify a Buckingham cutoff for an atom type pair, since only one global Buckingham cutoff is allowed. Similarly, if you are using *flag_coul* set to *long*, you cannot specify a Coulombic cutoff for an atom type pair, since only one global Coulombic cutoff is allowed.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair styles does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This pair style supports the *pair_modify* shift option for the energy of the exp() and 1/r^6 portion of the pair interaction, assuming *flag_buck* is *cut*.

This pair style does not support the *pair_modify* shift option for the energy of the Buckingham portion of the pair interaction.

This pair style supports the *pair_modify* table and table/disp options since they can tabulate the short-range portion of the long-range Coulombic and dispersion interactions.

This pair style write its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style supports the use of the *inner*, *middle*, and *outer* keywords of the *run_style respa* command, meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. See the *run_style* command for details.

18.59.4 Restrictions

This style is part of the KSPACE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.59.5 Related commands

pair_coeff

Default: none

(Ismail) Ismail, Tsige, In 't Veld, Grest, Molecular Physics (accepted) (2007).

18.60 pair_style lj/charmm/coul/charmm command

18.61 pair_style lj/charmm/coul/charmm/intel command

18.62 pair_style lj/charmm/coul/charmm/kk command

18.63 pair_style lj/charmm/coul/charmm/omp command

18.64 pair_style lj/charmm/coul/charmm/implicit command

18.65 pair_style lj/charmm/coul/charmm/implicit/kk command

18.66 pair_style lj/charmm/coul/charmm/implicit/omp command

18.67 pair_style lj/charmm/coul/long command

18.68 pair_style lj/charmm/coul/long/gpu command

18.69 pair_style lj/charmm/coul/long/intel command

18.70 pair_style lj/charmm/coul/long/kk command

18.71 pair_style lj/charmm/coul/long/opt command

18.72 pair_style lj/charmm/coul/long/omp command

18.73 pair_style lj/charmm/coul/msm command

18.74 pair_style lj/charmm/coul/msm/omp command

18.75 pair_style lj/charmmfsw/coul/charmmfsh command

18.76 pair_style lj/charmmfsw/coul/long command

18.76.1 Syntax

```
pair_style style args
```

- style = *lj/charmm/coul/charmm* or *lj/charmm/coul/charmm/implicit* or *lj/charmm/coul/long* or *lj/charmm/coul/msm* or *lj/charmmfsw/coul/charmmfsh* or *lj/charmmfsw/coul/long*

- args = list of arguments for a particular style

```
lj/charmm/coul/charmm args = inner outer (inner2) (outer2)
  inner, outer = global switching cutoffs for Lennard Jones (and Coulombic if␣
↪only 2 args)
  inner2, outer2 = global switching cutoffs for Coulombic (optional)
lj/charmm/coul/charmm/implicit args = inner outer (inner2) (outer2)
  inner, outer = global switching cutoffs for LJ (and Coulombic if only 2␣
↪args)
  inner2, outer2 = global switching cutoffs for Coulombic (optional)
lj/charmm/coul/long args = inner outer (cutoff)
  inner, outer = global switching cutoffs for LJ (and Coulombic if only 2␣
↪args)
  cutoff = global cutoff for Coulombic (optional, outer is Coulombic cutoff␣
↪if only 2 args)
lj/charmm/coul/msm args = inner outer (cutoff)
  inner, outer = global switching cutoffs for LJ (and Coulombic if only 2␣
↪args)
  cutoff = global cutoff for Coulombic (optional, outer is Coulombic cutoff␣
↪if only 2 args)
lj/charmmfsw/coul/charmmfsh args = inner outer (cutoff)
  inner, outer = global cutoffs for LJ (and Coulombic if only 2 args)
  cutoff = global cutoff for Coulombic (optional, outer is Coulombic cutoff␣
↪if only 2 args)
lj/charmmfsw/coul/long args = inner outer (cutoff)
  inner, outer = global cutoffs for LJ (and Coulombic if only 2 args)
  cutoff = global cutoff for Coulombic (optional, outer is Coulombic cutoff␣
↪if only 2 args)
```

18.76.2 Examples

```
pair_style lj/charmm/coul/charmm 8.0 10.0
pair_style lj/charmm/coul/charmm 8.0 10.0 7.0 9.0
pair_style lj/charmmfsw/coul/charmmfsh 10.0 12.0
pair_style lj/charmmfsw/coul/charmmfsh 10.0 12.0 9.0
pair_coeff * * 100.0 2.0
pair_coeff 1 1 100.0 2.0 150.0 3.5

pair_style lj/charmm/coul/charmm/implicit 8.0 10.0
pair_style lj/charmm/coul/charmm/implicit 8.0 10.0 7.0 9.0
pair_coeff * * 100.0 2.0
pair_coeff 1 1 100.0 2.0 150.0 3.5

pair_style lj/charmm/coul/long 8.0 10.0
pair_style lj/charmm/coul/long 8.0 10.0 9.0
pair_style lj/charmmfsw/coul/long 8.0 10.0
pair_style lj/charmmfsw/coul/long 8.0 10.0 9.0
pair_coeff * * 100.0 2.0
pair_coeff 1 1 100.0 2.0 150.0 3.5

pair_style lj/charmm/coul/msm 8.0 10.0
pair_style lj/charmm/coul/msm 8.0 10.0 9.0
pair_coeff * * 100.0 2.0
pair_coeff 1 1 100.0 2.0 150.0 3.5
```

18.76.3 Description

These pair styles compute Lennard Jones (LJ) and Coulombic interactions with additional switching or shifting functions that ramp the energy and/or force smoothly to zero between an inner and outer cutoff. They are implementations of the widely used CHARMM force field used in the CHARMM MD code (and others). See *(MacKerell)* for a description of the CHARMM force field.

The styles with *charmm* (not *charmmfsw* or *charmmfsh*) in their name are the older, original LAMMPS implementations. They compute the LJ and Coulombic interactions with an energy switching function (esw, shown in the formula below as S(r)), which ramps the energy smoothly to zero between the inner and outer cutoff. This can cause irregularities in pair-wise forces (due to the discontinuous 2nd derivative of energy at the boundaries of the switching region), which in some cases can result in detectable artifacts in an MD simulation.

The newer styles with *charmmfsw* or *charmmfsh* in their name replace the energy switching with force switching (fsw) and force shifting (fsh) functions, for LJ and Coulombic interactions respectively. These follow the formulas and description given in *(Steinbach)* and *(Brooks)* to minimize these artifacts.

Note: The newer *charmmfsw* or *charmmfsh* styles were released in March 2017. We recommend they be used instead of the older *charmm* styles. This includes the newer *dihedral_style charmmfsw* command. Eventually code from the new styles will propagate into the related pair styles (e.g. implicit, accelerator, free energy variants).

Note: The newest CHARMM pair styles reset the Coulombic energy conversion factor used internally in the code, from the LAMMPS value to the CHARMM value, as if it were effectively a parameter of the force field. This is because the CHARMM code uses a slightly different value for the this conversion factor in *real units* (Kcal/mole), namely CHARMM = 332.0716, LAMMPS = 332.06371. This is to enable more precise agreement by LAMMPS with the CHARMM force field energies and forces, when using one of these two CHARMM pair styles.

$$
\begin{aligned}
E =& LJ(r) && r < r_{\text{in}} \\
=& S(r) * LJ(r) && r_{\text{in}} < r < r_{\text{out}} \\
=& 0 && r > r_{\text{out}} \\
E =& C(r) && r < r_{\text{in}} \\
=& S(r) * C(r) && r_{\text{in}} < r < r_{\text{out}} \\
=& 0 && r > r_{\text{out}} \\
LJ(r) =& 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \\
C(r) =& \frac{C q_i q_j}{\epsilon r} \\
S(r) =& \frac{\left[r_{\text{out}}^2 - r^2\right]^2 \left[r_{\text{out}}^2 + 2r^2 - 3r_{\text{in}}^2\right]}{\left[r_{\text{out}}^2 - {r_{\text{in}}}^2\right]^3}
\end{aligned}
$$

where S(r) is the energy switching function mentioned above for the *charmm* styles. See the *(Steinbach)* paper for the functional forms of the force switching and force shifting functions used in the *charmmfsw* and *charmmfsh* styles.

When using the *lj/charmm/coul/charmm styles*, both the LJ and Coulombic terms require an inner and outer cutoff. They can be the same for both formulas or different depending on whether 2 or 4 arguments are used in the pair_style command. For the *lj/charmmfsw/coul/charmmfsh* style, the LJ term requires both an inner and outer cutoff, while the Coulombic term requires only one cutoff. If the Coulombic cutoff is not specified (2 instead of 3 arguments), the LJ outer cutoff is used for the Coulombic cutoff. In all cases where an inner and outer cutoff are specified, the inner cutoff distance must be less than the outer cutoff. It is typical to make the difference between the inner and outer cutoffs about 2.0 Angstroms.

Style *lj/charmm/coul/charmm/implicit* computes the same formulas as style *lj/charmm/coul/charmm* except that an additional 1/r term is included in the Coulombic formula. The Coulombic energy thus varies as 1/r^2. This is effectively a distance-dependent dielectric term which is a simple model for an implicit solvent with additional screening. It is designed for use in a simulation of an unsolvated biomolecule (no explicit water molecules).

Styles *lj/charmm/coul/long* and *lj/charmm/coul/msm* compute the same formulas as style *lj/charmm/coul/charmm* and style *lj/charmmfsw/coul/long* computes the same formulas as style *lj/charmmfsw/coul/charmmfsh*, except that an additional damping factor is applied to the Coulombic term, so it can be used in conjunction with the *kspace_style* command and its *ewald* or *pppm* or *msm* option. Only one Coulombic cutoff is specified for these styles; if only 2 arguments are used in the pair_style command, then the outer LJ cutoff is used as the single Coulombic cutoff. The Coulombic cutoff specified for these styles means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- ϵ (energy units)
- σ (distance units)
- ϵ_{14} (energy units)
- σ_{14} (distance units)

Note that σ is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum at $2^{1/6}\sigma$.

The latter 2 coefficients are optional. If they are specified, they are used in the LJ formula between 2 atoms of these types which are also first and fourth atoms in any dihedral. No cutoffs are specified because the CHARMM force field does not allow varying cutoffs for individual atom pairs; all pairs use the global cutoff(s) specified in the pair_style command.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon, sigma, epsilon_14, and sigma_14 coefficients for all of the lj/charmm pair styles can be mixed. The default mix value is *arithmetic* to coincide with the usual settings for the CHARMM force field. See the "pair_modify" command for details.

None of the *lj/charmm* or *lj/charmmfsw* pair styles support the *pair_modify* shift option, since the Lennard-Jones portion of the pair interaction is smoothed to 0.0 at the cutoff.

The *lj/charmm/coul/long* and *lj/charmmfsw/coul/long* styles support the *pair_modify* table option since they can tabulate the short-range portion of the long-range Coulombic interaction.

None of the *lj/charmm* or *lj/charmmfsw* pair styles support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure, since the Lennard-Jones portion of the pair interaction is smoothed to 0.0 at the cutoff.

All of the *lj/charmm* and *lj/charmmfsw* pair styles write their information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

The *lj/charmm/coul/long* and *lj/charmmfsw/coul/long* pair styles support the use of the *inner*, *middle*, and *outer* keywords of the *run_style respa* command, meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. The other styles only support the *pair* keyword of run_style respa. See the *run_style* command for details.

18.76.4 Restrictions

All the styles with *coul/charmm* or *coul/charmmfsh* styles are part of the MOLECULE package. All the styles with *coul/long* style are part of the KSPACE package. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

18.76.5 Related commands

pair_coeff

Default: none

(Brooks) Brooks, et al, J Comput Chem, 30, 1545 (2009).

(MacKerell) MacKerell, Bashford, Bellott, Dunbrack, Evanseck, Field, Fischer, Gao, Guo, Ha, et al, J Phys Chem, 102, 3586 (1998).

(Steinbach) Steinbach, Brooks, J Comput Chem, 15, 667 (1994).

18.77 pair_style lj/class2 command

18.78 pair_style lj/class2/gpu command

18.79 pair_style lj/class2/kk command

18.80 pair_style lj/class2/omp command

18.81 pair_style lj/class2/coul/cut command

18.82 pair_style lj/class2/coul/cut/kk command

18.83 pair_style lj/class2/coul/cut/omp command

18.84 pair_style lj/class2/coul/long command

18.85 pair_style lj/class2/coul/long/gpu command

18.86 pair_style lj/class2/coul/long/kk command

18.87 pair_style lj/class2/coul/long/omp command

18.87.1 Syntax

```
pair_style style args
```

- style = *lj/class2* or *lj/class2/coul/cut* or *lj/class2/coul/long*
- args = list of arguments for a particular style

```
lj/class2 args = cutoff
  cutoff = global cutoff for class 2 interactions (distance units)
lj/class2/coul/cut args = cutoff (cutoff2)
  cutoff = global cutoff for class 2 (and Coulombic if only 1 arg) (distance␣
↪units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
lj/class2/coul/long args = cutoff (cutoff2)
  cutoff = global cutoff for class 2 (and Coulombic if only 1 arg) (distance␣
↪units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
```

18.87.2 Examples

```
pair_style lj/class2 10.0
pair_coeff \* \* 100.0 2.5
pair_coeff 1 2\* 100.0 2.5 9.0

pair_style lj/class2/coul/cut 10.0
pair_style lj/class2/coul/cut 10.0 8.0
pair_coeff \* \* 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0
pair_coeff 1 1 100.0 3.5 9.0 9.0

pair_style lj/class2/coul/long 10.0
pair_style lj/class2/coul/long 10.0 8.0
pair_coeff \* \* 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0
```

18.87.3 Description

The *lj/class2* styles compute a 6/9 Lennard-Jones potential given by

$$E = \epsilon \left[2 \left(\frac{\sigma}{r} \right)^9 - 3 \left(\frac{\sigma}{r} \right)^6 \right] \qquad r < r_c$$

r_c is the cutoff.

The *lj/class2/coul/cut* and *lj/class2/coul/long* styles add a Coulombic term as described for the *lj/cut* pair styles.

See *(Sun)* for a description of the COMPASS class2 force field.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- ϵ (energy units)
- σ (distance units)
- cutoff1 (distance units)
- cutoff2 (distance units)

The latter 2 coefficients are optional. If not specified, the global class 2 and Coulombic cutoffs are used. If only one cutoff is specified, it is used as the cutoff for both class 2 and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the class 2 and Coulombic cutoffs for this type pair. You cannot specify 2 cutoffs for style *lj/class2*, since it has no Coulombic terms.

For *lj/class2/coul/long* only the class 2 cutoff can be specified since a Coulombic cutoff cannot be specified for an individual I,J type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

If the pair_coeff command is not used to define coefficients for a particular I != J type pair, the mixing rule for ϵ and σ for all class2 potentials is to use the *sixthpower* formulas documented by the *pair_modify* command. The *pair_modify mix* setting is thus ignored for class2 potentials for epsilon and sigma. However it is still followed for mixing the cutoff distance.

A version of these styles with a soft core, *lj/cut/soft*, suitable for use in free energy calculations, is part of the USER-FEP package and is documented with the *pair_style */soft* styles. The version with soft core is only available if LAMMPS was built with that package. See the *Build package* doc page for more info.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/class2 pair styles can be mixed. Epsilon and sigma are always mixed with the value *sixthpower*. The cutoff distance is mixed by whatever option is set by the pair_modify command (default = geometric). See the "pair_modify" command for details.

All of the lj/class2 pair styles support the *pair_modify* shift option for the energy of the Lennard-Jones portion of the pair interaction.

The *lj/class2/coul/long* pair style does not support the *pair_modify* table option since a tabulation capability has not yet been added to this potential.

All of the lj/class2 pair styles support the *pair_modify* tail option for adding a long-range tail correction to the energy and pressure of the Lennard-Jones portion of the pair interaction.

All of the lj/class2 pair styles write their information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

Only the *lj/class2* and *lj/class2/coul/long* pair styles support the use of the *inner*, *middle*, and *outer* keywords of the *run_style respa* command, meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. The other styles only support the *pair* keyword of run_style respa. See the *run_style* command for details.

18.87.4 Restrictions

These styles are part of the CLASS2 package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.87.5 Related commands

pair_coeff, *pair_style */soft*

Default: none

(Sun) Sun, J Phys Chem B 102, 7338-7364 (1998).

18.88 pair_style colloid command

18.89 pair_style colloid/gpu command

18.90 pair_style colloid/omp command

18.90.1 Syntax

```
pair_style colloid cutoff
```

- cutoff = global cutoff for colloidal interactions (distance units)

18.90.2 Examples

```
pair_style colloid 10.0
pair_coeff * *  25 1.0 10.0 10.0
pair_coeff 1 1 144 1.0 0.0 0.0 3.0
pair_coeff 1 2  75.398 1.0 0.0 10.0 9.0
pair_coeff 2 2  39.478 1.0 10.0 10.0 25.0
```

18.90.3 Description

Style *colloid* computes pairwise interactions between large colloidal particles and small solvent particles using 3 formulas. A colloidal particle has a size > sigma; a solvent particle is the usual Lennard-Jones particle of size sigma.

The colloid-colloid interaction energy is given by

$$U_A = -\frac{A_{cc}}{6}\left[\frac{2a_1a_2}{r^2-(a_1+a_2)^2}+\frac{2a_1a_2}{r^2-(a_1-a_2)^2}+\ln\left(\frac{r^2-(a_1+a_2)^2}{r^2-(a_1-a_2)^2}\right)\right]$$

$$\begin{aligned}U_R =& \frac{A_{cc}}{37800}\frac{\sigma^6}{r}\left[\frac{r^2-7r\left(a_1+a_2\right)+6\left(a_1^2+7a_1a_2+a_2^2\right)}{\left(r-a_1-a_2\right)^7}\right.\\ &+\frac{r^2+7r\left(a_1+a_2\right)+6\left(a_1^2+7a_1a_2+a_2^2\right)}{\left(r+a_1+a_2\right)^7}\\ &-\frac{r^2+7r\left(a_1-a_2\right)+6\left(a_1^2-7a_1a_2+a_2^2\right)}{\left(r+a_1-a_2\right)^7}\\ &\left.-\frac{r^2-7r\left(a_1-a_2\right)+6\left(a_1^2-7a_1a_2+a_2^2\right)}{\left(r-a_1+a_2\right)^7}\right]\end{aligned}$$

$$U = U_A + U_R, \qquad r < r_c$$

where A_{cc} is the Hamaker constant, a_1 and a_2 are the radii of the two colloidal particles, and r_c is the cutoff. This equation results from describing each colloidal particle as an integrated collection of Lennard-Jones particles of size sigma and is derived in *(Everaers)*.

The colloid-solvent interaction energy is given by

$$U = \frac{2\,a^3\,\sigma^3\,A_{cs}}{9\left(a^2-r^2\right)^3}\left[1-\frac{\left(5\,a^6+45\,a^4\,r^2+63\,a^2\,r^4+15\,r^6\right)\sigma^6}{15\left(a-r\right)^6\left(a+r\right)^6}\right], \quad r<r_c$$

where :math:A_{cs}` is the Hamaker constant, a is the radius of the colloidal particle, and r_c is the cutoff. This formula is derived from the colloid-colloid interaction, letting one of the particle sizes go to zero.

The solvent-solvent interaction energy is given by the usual Lennard-Jones formula

$$U = \frac{A_{ss}}{36}\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right], \quad r<r_c$$

with A_{ss} set appropriately, which results from letting both particle sizes go to zero.

When used in combination with *pair_style yukawa/colloid*, the two terms become the so-called DLVO potential, which combines electrostatic repulsion and van der Waals attraction.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- A (energy units)
- σ (distance units)
- d1 (distance units)
- d2 (distance units)
- cutoff (distance units)

A is the Hamaker energy prefactor and should typically be set as follows:

- A_{cc} = colloid/colloid = $4\pi^2 = 39.5$
- A_{cs} = colloid/solvent = $\sqrt{A_{cc}A_{ss}}$
- A_{ss} = solvent/solvent = 144 (assuming epsilon = 1, so that 144/36 = 4)

σ is the size of the solvent particle or the constituent particles integrated over in the colloidal particle and should typically be set as follows:

- σ_{cc} = colloid/colloid = 1.0
- σ_{cs} = colloid/solvent = arithmetic mixing between colloid σ and solvent σ
- σ_{ss} = solvent/solvent = 1.0 or whatever size the solvent particle is

Thus typically $\sigma_{cs} = 1.0$, unless the solvent particle's size != 1.0.

D1 and d2 are particle diameters, so that d1 = 2*a1 and d2 = 2*a2 in the formulas above. Both d1 and d2 must be values >= 0. If d1 > 0 and d2 > 0, then the pair interacts via the colloid-colloid formula above. If d1 = 0 and d2 = 0, then the pair interacts via the solvent-solvent formula. I.e. a d value of 0 is a Lennard-Jones particle of size σ. If either d1 = 0 or d2 = 0 and the other is larger, then the pair interacts via the colloid-solvent formula.

Note that the diameter of a particular particle type may appear in multiple pair_coeff commands, as it interacts with other particle types. You should insure the particle diameter is specified consistently each time it appears.

The last coefficient is optional. If not specified, the global cutoff specified in the pair_style command is used. However, you typically want different cutoffs for interactions between different particle sizes. E.g. if colloidal particles of diameter 10 are used with solvent particles of diameter 1, then a solvent-solvent cutoff of 2.5 would correspond to a colloid-colloid cutoff of 25. A good rule-of-thumb is to use a colloid-solvent cutoff that is half the big diameter + 4 times the small diameter. I.e. 9 = 5 + 4 for the colloid-solvent cutoff in this case.

Note: When using pair_style colloid for a mixture with 2 (or more) widely different particles sizes (e.g. sigma=10 colloids in a background sigma=1 LJ fluid), you will likely want to use these commands for efficiency: *neighbor multi* and *comm_modify multi*.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the A, sigma, d1, and d2 coefficients and cutoff distance for this pair style can be mixed. A is an energy value mixed like a LJ epsilon. D1 and d2 are distance values and are mixed like sigma. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style supports the *pair_modify* shift option for the energy of the pair interaction.

The *pair_modify* table option is not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.90.4 Restrictions

This style is part of the COLLOID package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Normally, this pair style should be used with finite-size particles which have a diameter, e.g. see the *atom_style sphere* command. However, this is not a requirement, since the only definition of particle size is via the pair_coeff parameters for each type. In other words, the physical radius of the particle is ignored. Thus you should insure that the d1,d2 parameters you specify are consistent with the physical size of the particles of that type.

Per-particle polydispersity is not yet supported by this pair style; only per-type polydispersity is enabled via the pair_coeff parameters.

18.90.5 Related commands

pair_coeff

Default: none

(Everaers) Everaers, Ejtehadi, Phys Rev E, 67, 041710 (2003).

18.91 pair_style comb command

18.92 pair_style comb/omp command

18.93 pair_style comb3 command

18.93.1 Syntax

```
pair_style comb
pair_style comb3 keyword
```

```
keyword = polar
  polar value = polar_on or polar_off = whether or not to include atomic␣
↪polarization
```

18.93.2 Examples

```
pair_style comb
pair_coeff * * ../potentials/ffield.comb Si
pair_coeff * * ../potentials/ffield.comb Hf Si O

pair_style comb3 polar_off
pair_coeff * * ../potentials/ffield.comb3 O Cu N C O
```

18.93.3 Description

Style *comb* computes the second-generation variable charge COMB (Charge-Optimized Many-Body) potential. Style *comb3* computes the third-generation COMB potential. These COMB potentials are described in *(COMB)* and *(COMB3)*. Briefly, the total energy E_T of a system of atoms is given by

$$E_T = \sum_i [E_i^{self}(q_i) + \sum_{j>i} [E_{ij}^{short}(r_{ij}, q_i, q_j) + E_{ij}^{Coul}(r_{ij}, q_i, q_j)] + E^{polar}(q_i, r_{ij}) + E^{vdW}(r_{ij}) + E^{barr}(q_i) + E^{corr}(r_{ij}, \theta_{jik})]$$

where E_i^{self} is the self-energy of atom *i* (including atomic ionization energies and electron affinities), E_{ij}^{short} is the bond-order potential between atoms *i* and *j*, E_{ij}^{Coul} is the Coulomb interactions, E^{polar} is the polarization term for organic systems (style *comb3* only), E^{vdW} is the van der Waals energy (style *comb3* only), E^{barr} is a charge barrier function, and E^{corr} are angular correction terms.

The COMB potentials (styles *comb* and *comb3*) are variable charge potentials. The equilibrium charge on each atom is calculated by the electronegativity equalization (QEq) method. See *Rick* for further details. This is implemented by the *fix qeq/comb* command, which should normally be specified in the input script when running a model with the COMB potential. The *fix qeq/comb* command has options that determine how often charge equilibration is performed, its convergence criterion, and which atoms are included in the calculation.

Only a single pair_coeff command is used with the *comb* and *comb3* styles which specifies the COMB potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the potential file in the pair_coeff command, where N is the number of LAMMPS atom types.

For example, if your LAMMPS simulation of a Si/SiO2/ HfO2 interface has 4 atom types, and you want the 1st and last to be Si, the 2nd to be Hf, and the 3rd to be O, and you would use the following pair_coeff command:

```
pair_coeff * * ../potentials/ffield.comb Si Hf O Si
```

The first two arguments must be * * so as to span all LAMMPS atom types. The first and last Si arguments map LAMMPS atom types 1 and 4 to the Si element in the *ffield.comb* file. The second Hf argument maps LAMMPS atom type 2 to the Hf element, and the third O argument maps LAMMPS atom type 3 to the O element in the potential file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *comb* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

For style *comb*, the provided potential file *ffield.comb* contains all currently-available 2nd generation COMB parameterizations: for Si, Cu, Hf, Ti, O, their oxides and Zr, Zn and U metals. For style *comb3*, the potential file *ffield.comb3* contains all currently-available 3rd generation COMB parameterizations: O, Cu, N, C, H, Ti, Zn and Zr. The status of the optimization of the compounds, for example Cu2O, TiN and hydrocarbons, are given in the following table:

	O	Cu	N	C	H	Ti	Zn	Zr
O	F	F	F	F	F	F	F	F
Cu	F	F	P	F	F	P	F	P
N	F	P	F	M	F	P	P	P
C	F	F	M	F	F	M	M	M
H	F	F	F	F	F	M	M	F
Ti	F	P	P	M	M	F	P	P
Zn	F	F	P	M	M	P	F	P
Zr	F	P	P	M	F	P	P	F

- F = Fully optimized
- M = Only optimized for dimer molecule
- P = in progress, but have it from mixing rule

For style *comb3*, in addition to ffield.comb3, a special parameter file, *lib.comb3*, that is exclusively used for C/O/H systems, will be automatically loaded if carbon atom is detected in LAMMPS input structure. This file must be in your working directory or in the directory pointed to by the environment variable LAMMPS_POTENTIALS, as described on the *pair_coeff* command doc page.

Keyword *polar* indicates whether the force field includes the atomic polarization. Since the equilibration of the polarization has not yet been implemented, it can only set polar_off at present.

Note: You can not use potential file *ffield.comb* with style *comb3*, nor file *ffield.comb3* with style *comb*.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages*

doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above from values in the potential file.

These pair styles does not support the *pair_modify* shift, table, and tail options.

These pair styles do not write its information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style, pair_coeff, and *fix qeq/comb* commands in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.93.4 Restrictions

These pair styles are part of the MANYBODY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

These pair styles requires the *newton* setting to be "on" for pair interactions.

The COMB potentials in the *ffield.comb* and *ffield.comb3* files provided with LAMMPS (see the potentials directory) are parameterized for metal *units*. You can use the COMB potential with any LAMMPS units, but you would need to create your own COMB potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

18.93.5 Related commands

pair_style, *pair_coeff*, *fix qeq/comb*

Default: none

(COMB) T.-R. Shan, B. D. Devine, T. W. Kemper, S. B. Sinnott, and S. R. Phillpot, Phys. Rev. B 81, 125328 (2010)

(COMB3) T. Liang, T.-R. Shan, Y.-T. Cheng, B. D. Devine, M. Noordhoek, Y. Li, Z. Lu, S. R. Phillpot, and S. B. Sinnott, Mat. Sci. & Eng: R 74, 255-279 (2013).

(Rick) S. W. Rick, S. J. Stuart, B. J. Berne, J Chem Phys 101, 6141 (1994).

18.94 pair_style cosine/squared command

18.94.1 Syntax

```
pair_style cosine/squared cutoff
```

- cutoff = global cutoff for cosine-squared interactions (distance units)

```
pair_coeff i j eps sigma
pair_coeff i j eps sigma cutoff
pair_coeff i j eps sigma wca
pair_coeff i j eps sigma cutoff wca
```

- i,j = a particle type
- eps = interaction strength, i.e. the depth of the potential minimum (energy units)
- sigma = distance of the potential minimum from 0
- cutoff = the cutoff distance for this pair type, if different from global (distance units)
- wca = if specified a Weeks-Chandler-Andersen potential (with eps strength and minimum at sigma) is added, otherwise not

18.94.2 Examples

```
pair_style cosine/squared 3.0
pair_coeff * * 1.0 1.3
pair_coeff 1 3 1.0 1.3 2.0
pair_coeff 1 3 1.0 1.3 wca
pair_coeff 1 3 1.0 1.3 2.0 wca
```

18.94.3 Description

Style *cosine/squared* computes a potential of the form

$$E = \begin{cases} -\epsilon & r < \sigma \\ -\epsilon \cos\left(\frac{\pi(r-\sigma)}{2(r_c-\sigma)}\right) & \sigma \leq r < r_c \\ 0 & r \geq r_c \end{cases}$$

between two point particles, where $(\sigma, -\epsilon)$ is the location of the (rightmost) minimum of the potential, as explained in the syntax section above.

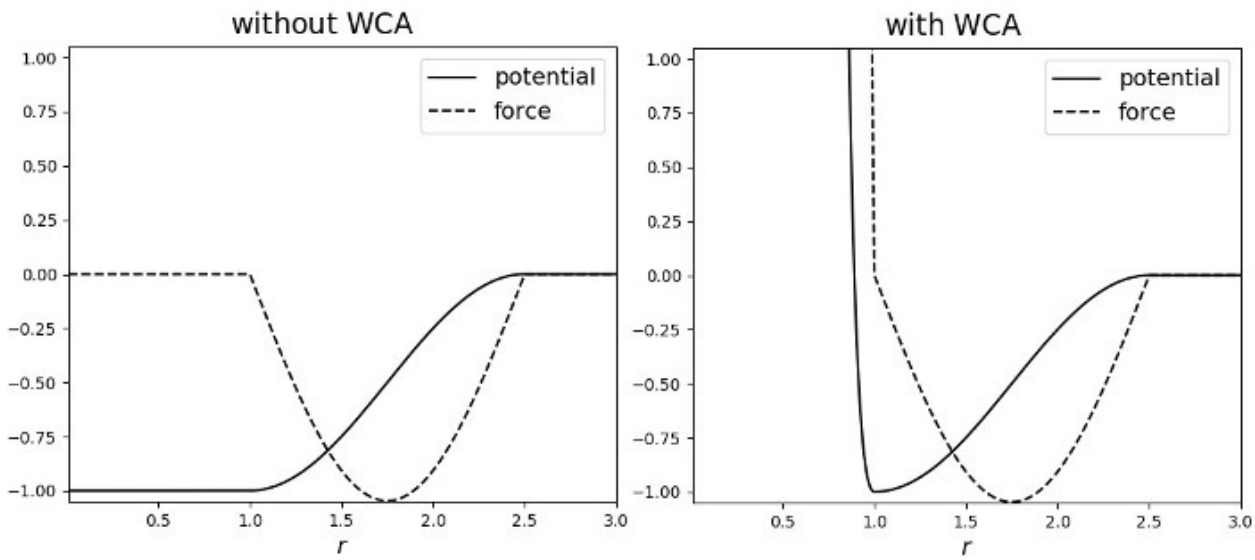
This potential was first used in (Cooke)_#CKD for a coarse-grained lipid membrane model. It is generally very useful as a non-specific interaction potential because it is fully adjustable in depth and width while joining the minimum at (sigma, -epsilon) and zero at (cutoff, 0) smoothly, requiring no shifting and causing no related artifacts, tail energy calculations etc. This evidently requires *cutoff* to be larger than *sigma*.

If the *wca* option is used then a Weeks-Chandler-Andersen potential (Weeks)_#WCA is added to the above specified cosine-squared potential, specifically the following:

$$E = \epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - 2\left(\frac{\sigma}{r}\right)^{6} + 1 \right], \quad r < \sigma$$

In this case, and this case only, the σ parameter can be equal to *cutoff* (σ = cutoff) which will result in ONLY the WCA potential being used (and print a warning), so the minimum will be attained at (sigma, 0). This is a convenience feature that enables a purely repulsive potential to be used without a need to define an additional pair style and use the hybrid styles.

The energy and force of this pair style for parameters epsilon = 1.0, sigma = 1.0, cutoff = 2.5, with and without the WCA potential, are shown in the graphs below:



Mixing, shift, table, tail correction, restart, rRESPA info:

Mixing is not supported for this style.

The *shift*, *table* and *tail* options are not relevant for this style.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

18.94.4 Restrictions

The *cosine/squared* style is part of the "USER-MISC" package. It is only enabled if LAMMPS is build with that package. See the *Build package* doc page for more info.

18.94.5 Related commands

pair_coeff, *pair_style lj/cut*

Default: none

(Cooke) "Cooke, Kremer and Deserno, Phys. Rev. E, 72, 011506 (2005)"

(Weeks) "Weeks, Chandler and Andersen, J. Chem. Phys., 54, 5237 (1971)"

18.95 pair_style coul/cut command

18.96 pair_style coul/cut/gpu command

18.97 pair_style coul/cut/kk command

18.98 pair_style coul/cut/omp command

18.99 pair_style coul/debye command

18.100 pair_style coul/debye/gpu command

18.101 pair_style coul/debye/kk command

18.102 pair_style coul/debye/omp command

18.103 pair_style coul/dsf command

18.104 pair_style coul/dsf/gpu command

18.105 pair_style coul/dsf/kk command

18.106 pair_style coul/dsf/omp command

18.107 pair_style coul/long command

18.108 pair_style coul/long/omp command

18.109 pair_style coul/long/gpu command

18.110 pair_style coul/long/kk command

18.111 pair_style coul/msm command

18.112 pair_style coul/msm/omp command

18.113 pair_style coul/streitz command

18.114 pair_style coul/wolf command

18.115 pair_style coul/wolf/kk command

18.116 pair_style coul/wolf/omp command

```
pair_style coul/cut cutoff
pair_style coul/debye kappa cutoff
pair_style coul/dsf alpha cutoff
pair_style coul/long cutoff
pair_style coul/long/gpu cutoff
pair_style coul/wolf alpha cutoff
pair_style coul/streitz cutoff keyword alpha
pair_style tip4p/cut otype htype btype atype qdist cutoff
pair_style tip4p/long otype htype btype atype qdist cutoff
```

- cutoff = global cutoff for Coulombic interactions
- kappa = Debye length (inverse distance units)
- alpha = damping parameter (inverse distance units)

18.120.2 Examples

```
pair_style coul/cut 2.5
pair_coeff * *
pair_coeff 2 2 3.5

pair_style coul/debye 1.4 3.0
pair_coeff * *
pair_coeff 2 2 3.5

pair_style coul/dsf 0.05 10.0
pair_coeff * *

pair_style coul/long 10.0
pair_coeff * *

pair_style coul/msm 10.0
pair_coeff * *

pair_style coul/wolf 0.2 9.0
pair_coeff * *

pair_style coul/streitz 12.0 ewald
pair_style coul/streitz 12.0 wolf 0.30
pair_coeff * * AlO.streitz Al O

pair_style tip4p/cut 1 2 7 8 0.15 12.0
pair_coeff * *

pair_style tip4p/long 1 2 7 8 0.15 10.0
pair_coeff * *
```

18.120.3 Description

The *coul/cut* style computes the standard Coulombic interaction potential given by

$$E = \frac{Cq_iq_j}{\epsilon r} \qquad r < r_c$$

where C is an energy-conversion constant, Qi and Qj are the charges on the 2 atoms, and ϵ is the dielectric constant which can be set by the *dielectric* command. The cutoff r_c truncates the interaction distance.

Style *coul/debye* adds an additional exp() damping factor to the Coulombic term, given by

$$E = \frac{Cq_iq_j}{\epsilon r} \exp(-\kappa r) \qquad r < r_c$$

where κ is the Debye length. This potential is another way to mimic the screening effect of a polar solvent.

Style *coul/dsf* computes Coulombic interactions via the damped shifted force model described in *Fennell*, given by:

$$E = q_iq_j \left[\frac{\mathrm{erfc}(\alpha r)}{r} - \frac{\mathrm{erfc}(\alpha r_c)}{r_c} + \left(\frac{\mathrm{erfc}(\alpha r_c)}{r_c^2} + \frac{2\alpha}{\sqrt{\pi}} \frac{\exp(-\alpha^2 r_c^2)}{r_c} \right) (r - r_c) \right] \qquad r < r_c$$

where α is the damping parameter and erfc() is the complementary error-function. The potential corrects issues in the Wolf model (described below) to provide consistent forces and energies (the Wolf potential is not differentiable at the cutoff) and smooth decay to zero.

Style *coul/wolf* computes Coulombic interactions via the Wolf summation method, described in *Wolf*, given by:

$$E_i = \frac{1}{2} \sum_{j \neq i} \frac{q_iq_j \mathrm{erfc}(\alpha r_{ij})}{r_{ij}} + \frac{1}{2} \sum_{j \neq i} \frac{q_iq_j \mathrm{erf}(\alpha r_{ij})}{r_{ij}} \qquad r < r_c$$

where α is the damping parameter, and erc() and erfc() are error-function and complementary error-function terms. This potential is essentially a short-range, spherically-truncated, charge-neutralized, shifted, pairwise *1/r* summation. With a manipulation of adding and subtracting a self term (for i = j) to the first and second term on the right-hand-side, respectively, and a small enough α damping parameter, the second term shrinks and the potential becomes a rapidly-converging real-space summation. With a long enough cutoff and small enough α parameter, the energy and forces calculated by the Wolf summation method approach those of the Ewald sum. So it is a means of getting effective long-range interactions with a short-range potential.

Style *coul/streitz* is the Coulomb pair interaction defined as part of the Streitz-Mintmire potential, as described in *this paper*, in which charge distribution about an atom is modeled as a Slater 1*s* orbital. More details can be found in the referenced paper. To fully reproduce the published Streitz-Mintmire potential, which is a variable charge potential, style *coul/streitz* must be used with *pair_style eam/alloy* (or some other short-range potential that has been parameterized appropriately) via the *pair_style hybrid/overlay* command. Likewise, charge equilibration must be performed via the *fix qeq/slater* command. For example:

```
pair_style hybrid/overlay coul/streitz 12.0 wolf 0.31 eam/alloy
pair_coeff * * coul/streitz AlO.streitz Al O
pair_coeff * * eam/alloy AlO.eam.alloy Al O
fix 1 all qeq/slater 1 12.0 1.0e-6 100 coul/streitz
```

The keyword *wolf* in the coul/streitz command denotes computing Coulombic interactions via Wolf summation. An additional damping parameter is required for the Wolf summation, as described for the coul/wolf potential above. Alternatively, Coulombic interactions can be computed via an Ewald summation. For example:

```
pair_style hybrid/overlay coul/streitz 12.0 ewald eam/alloy
kspace_style ewald 1e-6
```

Keyword *ewald* does not need a damping parameter, but a *kspace_style* must be defined, which can be style *ewald* or *pppm*. The Ewald method was used in Streitz and Mintmire's original paper, but a Wolf summation offers a speed-up in some cases.

For the fix qeq/slater command, the *qfile* can be a filename that contains QEq parameters as discussed on the *fix qeq* command doc page. Alternatively *qfile* can be replaced by "coul/streitz", in which case the fix will extract QEq parameters from the coul/streitz pair style itself.

See the examples/strietz directory for an example input script that uses the Streitz-Mintmire potential. The potentials directory has the AlO.eam.alloy and AlO.streitz potential files used by the example.

Note that the Streiz-Mintmire potential is generally used for oxides, but there is no conceptual problem with extending it to nitrides and carbides (such as SiC, TiN). Pair coul/strietz used by itself or with any other pair style such as EAM, MEAM, Tersoff, or LJ in hybrid/overlay mode. To do this, you would need to provide a Streitz-Mintmire parameterization for the material being modeled.

Styles *coul/long* and *coul/msm* compute the same Coulombic interactions as style *coul/cut* except that an additional damping factor is applied so it can be used in conjunction with the *kspace_style* command and its *ewald* or *pppm* option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

Styles *tip4p/cut* and *tip4p/long* implement the Coulomb part of the TIP4P water model of *(Jorgensen)*, which introduces a massless site located a short distance away from the oxygen atom along the bisector of the HOH angle. The atomic types of the oxygen and hydrogen atoms, the bond and angle types for OH and HOH interactions, and the distance to the massless charge site are specified as pair_style arguments. Style *tip4p/cut* uses a global cutoff for Coulomb interactions; style *tip4p/long* is for use with a long-range Coulombic solver (Ewald or PPPM).

Note: For each TIP4P water molecule in your system, the atom IDs for the O and 2 H atoms must be consecutive, with the O atom first. This is to enable LAMMPS to "find" the 2 H atoms associated with each O atom. For example, if the atom ID of an O atom in a TIP4P water molecule is 500, then its 2 H atoms must have IDs 501 and 502.

See the *Howto tip4p* doc page for more information on how to use the TIP4P pair styles and lists of parameters to set. Note that the neighbor list cutoff for Coulomb interactions is effectively extended by a distance 2*qdist when using the TIP4P pair style, to account for the offset distance of the fictitious charges on O atoms in water molecules. Thus it is typically best in an efficiency sense to use a LJ cutoff >= Coulombic cutoff + 2*qdist, to shrink the size of the neighbor list. This leads to slightly larger cost for the long-range calculation, so you can test the trade-off for your model.

Note that these potentials are designed to be combined with other pair potentials via the *pair_style hybrid/overlay* command. This is because they have no repulsive core. Hence if they are used by themselves, there will be no repulsion to keep two oppositely charged particles from moving arbitrarily close to each other.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- cutoff (distance units)

For *coul/cut* and *coul/debye*, the cutoff coefficient is optional. If it is not used (as in some of the examples above), the default global value specified in the pair_style command is used.

For *coul/long* and *coul/msm* no cutoff can be specified for an individual I,J type pair via the pair_coeff command. All type pairs use the same global Coulomb cutoff specified in the pair_style command.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the cutoff distance for the *coul/cut* style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

The *pair_modify* shift option is not relevant for these pair styles.

The *coul/long* style supports the *pair_modify* table option for tabulation of the short-range portion of the long-range Coulombic interaction.

These pair styles do not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

These pair styles write their information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

18.120.4 Restrictions

The *coul/long*, *coul/msm* and *tip4p/long* styles are part of the KSPACE package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.120.5 Related commands

pair_coeff, *pair_style, hybrid/overlay*, *kspace_style*

Default: none

(Wolf) D. Wolf, P. Keblinski, S. R. Phillpot, J. Eggebrecht, J Chem Phys, 110, 8254 (1999).

(Fennell) C. J. Fennell, J. D. Gezelter, J Chem Phys, 124, 234104 (2006).

(Streitz) F. H. Streitz, J. W. Mintmire, Phys Rev B, 50, 11996-12003 (1994).

(Jorgensen) Jorgensen, Chandrasekhar, Madura, Impey, Klein, J Chem Phys, 79, 926 (1983).

18.121 pair_style coul/diel command

18.122 pair_style coul/diel/omp command

18.122.1 Syntax

```
pair_style coul/diel cutoff
```

cutoff = global cutoff (distance units)

18.122.2 Examples

```
pair_style coul/diel 3.5
pair_coeff 1 4 78. 1.375 0.112
```

18.122.3 Description

Style *coul/diel* computes a Coulomb correction for implicit solvent ion interactions in which the dielectric permittivity is distance dependent. The dielectric permittivity epsilon_D(r) connects to limiting regimes: One limit is defined by a small dielectric permittivity (close to vacuum) at or close to contact separation between the ions. At larger separations the dielectric permittivity reaches a bulk value used in the regular Coulomb interaction coul/long or coul/cut. The transition is modeled by a hyperbolic function which is incorporated in the Coulomb correction term for small ion separations as follows

$$E = \frac{C q_i q_j}{\epsilon r} \left(\frac{\epsilon}{\epsilon_D(r)} - 1 \right) \qquad r < r_c$$
$$\epsilon_D(r) = \frac{5.2 + \epsilon}{2} + \frac{\epsilon - 5.2}{2} \tanh \left(\frac{r - r_{me}}{\sigma_e} \right)$$

where r_{me} is the inflection point of $\epsilon_D(r)$ and σ_e is a slope defining length scale. C is the same Coulomb conversion factor as in the pair_styles coul/cut, coul/long, and coul/debye. In this way the Coulomb interaction between ions is corrected at small distances r. The lower limit of epsilon_D(r->0)=5.2 due to dielectric saturation *(Stiles)* while the Coulomb interaction reaches its bulk limit by setting $\epsilon_D(r \to \infty) = \epsilon$, the bulk value of the solvent which is 78 for water at 298K.

Examples of the use of this type of Coulomb interaction include implicit solvent simulations of salt ions *(Lenart)* and of ionic surfactants *(Jusufi)*. Note that this potential is only reasonable for implicit solvent simulations and in combination with coul/cut or coul/long. It is also usually combined with gauss/cut, see *(Lenart)* or *(Jusufi)*.

The following coefficients must be defined for each pair of atom types via the *pair_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- ϵ (no units)
- r_{me} (distance units)
- σ_e (distance units)

The global cutoff (r_c) specified in the pair_style command is used.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support parameter mixing. Coefficients must be given explicitly for each type of particle pairs.

This pair style supports the *pair_modify* shift option for the energy of the Gauss-potential portion of the pair interaction.

The *pair_modify* table option is not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.122.4 Restrictions

This style is part of the "USER-MISC" package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.122.5 Related commands

pair_coeff pair_style gauss/cut

Default: none

(Stiles) Stiles , Hubbard, and Kayser, J Chem Phys, 77, 6189 (1982).

(Lenart) Lenart , Jusufi, and Panagiotopoulos, J Chem Phys, 126, 044509 (2007).

(Jusufi) Jusufi, Hynninen, and Panagiotopoulos, J Phys Chem B, 112, 13783 (2008).

18.123 pair_style coul/shield command

18.123.1 Syntax

```
pair_style coul/shield cutoff tap_flag
```

- cutoff = global cutoff (distance units)
- tap_flag = 0/1 to turn off/on the taper function

18.123.2 Examples

```
pair_style coul/shield 16.0 1
pair_coeff 1 2 0.70
```

18.123.3 Description

Style *coul/shield* computes a Coulomb interaction for boron and nitrogen atoms located in different layers of hexagonal boron nitride. This potential is designed be used in combination with the pair style *ilp/graphene/hbn*

Note: This potential is intended for electrostatic interactions between two different layers of hexagonal boron nitride. Therefore, to avoid interaction within the same layers, each layer should have a separate molecule id and is recommended to use the "full" atom style, so that charge and molecule ID information is included.

$$
\begin{aligned}
E =& \frac{1}{2} \sum_i \sum_{j \neq i} V_{ij} \\
V_{ij} =& \mathrm{Tap}(r_{ij}) \frac{\kappa q_i q_j}{\sqrt[3]{r_{ij}^3 + (1/\lambda_{ij})^3}} \\
\mathrm{Tap}(r_{ij}) =& 20 \left(\frac{r_{ij}}{R_{cut}}\right)^7 - 70 \left(\frac{r_{ij}}{R_{cut}}\right)^6 + 84 \left(\frac{r_{ij}}{R_{cut}}\right)^5 - 35 \left(\frac{r_{ij}}{R_{cut}}\right)^4 + 1
\end{aligned}
$$

Where Tap(r_{ij}) is the taper function which provides a continuous cutoff (up to third derivative) for inter-atomic separations larger than r_c *(Leven1)*, *(Leven2)* and *(Maaravi)*. Here λ is the shielding parameter that eliminates the short-range singularity of the classical mono-polar electrostatic interaction expression *(Maaravi)*.

The shielding parameter λ (1/distance units) must be defined for each pair of atom types via the *pair_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

The global cutoff (r_c) specified in the pair_style command is used.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support parameter mixing. Coefficients must be given explicitly for each type of particle pairs.

The *pair_modify table* option is not relevant for this pair style.

This pair style does not support the *pair_modify tail* option for adding long-range tail corrections to energy and pressure.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.123.4 Restrictions

This style is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.123.5 Related commands

pair_coeff pair_style ilp/graphene/hbn

Default: tap_flag = 1

(Leven1) I. Leven, I. Azuri, L. Kronik and O. Hod, J. Chem. Phys. 140, 104106 (2014).

(Leven2) I. Leven et al, J. Chem.Theory Comput. 12, 2896-905 (2016).

(Maaravi) T. Maaravi et al, J. Phys. Chem. C 121, 22826-22835 (2017).

18.124 pair_style born/coul/dsf/cs command

18.125 pair_style born/coul/long/cs command

18.126 pair_style born/coul/long/cs/gpu command

18.127 pair_style born/coul/wolf/cs command

18.128 pair_style born/coul/wolf/cs/gpu command

18.129 pair_style buck/coul/long/cs command

18.130 pair_style coul/long/cs command

18.131 pair_style coul/long/cs/gpu command

18.132 pair_style coul/wolf/cs command

18.133 pair_style lj/cut/coul/long/cs command

18.133.1 Syntax

```
pair_style style args
```

- style = *born/coul/dsf/cs* or *born/coul/long/cs* or *born/coul/wolf/cs* or *buck/coul/long/cs* or *coul/long/cs* or *coul/wolf/cs* or *lj/cut/coul/long/cs*
- args = list of arguments for a particular style

```
born/coul/dsf/cs args = alpha cutoff (cutoff2)
  alpha = damping parameter (inverse distance units)
  cutoff = global cutoff for non-Coulombic (and Coulombic if only 1 arg)␣
↪(distance units)
  cutoff2 = global cutoff for Coulombic (distance units)
```

```
born/coul/long/cs args = cutoff (cutoff2)
  cutoff = global cutoff for non-Coulombic (and Coulombic if only 1 arg)␣
↪(distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
born/coul/wolf/cs args = alpha cutoff (cutoff2)
  alpha = damping parameter (inverse distance units)
  cutoff = global cutoff for Buckingham (and Coulombic if only 1 arg)␣
↪(distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
buck/coul/long/cs args = cutoff (cutoff2)
  cutoff = global cutoff for Buckingham (and Coulombic if only 1 arg)␣
↪(distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
coul/long args = cutoff
  cutoff = global cutoff for Coulombic (distance units)
coul/wolf args = alpha cutoff
  alpha = damping parameter (inverse distance units)
  cutoff = global cutoff for Coulombic (distance units)
lj/cut/coul/long/cs args = cutoff (cutoff2)
  cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
```

18.133.2 Examples

```
pair_style born/coul/dsf/cs 0.1 10.0 12.0
pair_coeff * *   0.0 1.00 0.00 0.00 0.00
pair_coeff 1 1 480.0 0.25 0.00 1.05 0.50

pair_style born/coul/long/cs 10.0 8.0
pair_coeff 1 1 6.08 0.317 2.340 24.18 11.51

pair_style born/coul/wolf/cs 0.25 10.0 12.0
pair_coeff * *   0.0 1.00 0.00 0.00 0.00
pair_coeff 1 1 480.0 0.25 0.00 1.05 0.50

pair_style buck/coul/long/cs 10.0
pair_style buck/coul/long/cs 10.0 8.0
pair_coeff * * 100.0 1.5 200.0
pair_coeff 1 1 100.0 1.5 200.0 9.0

pair_style coul/long/cs 10.0
pair_coeff * *

pair_style coul/wolf/cs 0.2 9.0
pair_coeff * *

pair_style lj/cut/coul/long/cs 10.0
pair_style lj/cut/coul/long/cs 10.0 8.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0
```

18.133.3 Description

These pair styles are designed to be used with the adiabatic core/shell model of *(Mitchell and Finchham)*. See the *Howto coreshell* doc page for an overview of the model as implemented in LAMMPS.

All the styles are identical to the corresponding pair style without the "/cs" in the name:

- *pair_style born/coul/dsf*
- *pair_style born/coul/long*
- *pair_style born/coul/wolf*
- *pair_style buck/coul/long*
- *pair_style coul/long*
- *pair_style coul/wolf*
- *pair_style lj/cut/coul/long*

except that they correctly treat the special case where the distance between two charged core and shell atoms in the same core/shell pair approach r = 0.0.

Styles with a "/long" in the name are used with a long-range solver for Coulombic interactions via the *kspace_style* command. They require special treatment of the short-range Coulombic interactions within the cor/shell model.

Specifically, the short-range Coulomb interaction between a core and its shell should be turned off using the *special_bonds* command by setting the 1-2 weight to 0.0, which works because the core and shell atoms are bonded to each other. This induces a long-range correction approximation which fails at small distances (~< 10e-8). Therefore, the Coulomb term which is used to calculate the correction factor is extended by a minimal distance (r_min = 1.0-6) when the interaction between a core/shell pair is treated, as follows

$$E = \frac{C q_i q_j}{\epsilon(r + r_{min})} \qquad r \to 0$$

where C is an energy-conversion constant, q_i and q_j are the charges on the core and shell, epsilon is the dielectric constant and r_{min} is the minimal distance.

For styles that are not used with a long-range solver, i.e. those with "/dsf" or "/wolf" in the name, the only correction is the addition of a minimal distance to avoid the possible r = 0.0 case for a core/shell pair.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

See the corresponding doc pages for pair styles without the "cs" suffix to see how mixing, shifting, tabulation, tail correction, restarting, and rRESPA are handled by theses pair styles.

18.133.4 Restrictions

These pair styles are part of the CORESHELL package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.133.5 Related commands

pair_coeff, *pair_style born*, *pair_style buck*

Default: none

(Mitchell and Finchham) Mitchell, Finchham, J Phys Condensed Matter, 5, 1031-1038 (1993).

18.134 pair_style lj/cut/dipole/cut command

18.135 pair_style lj/cut/dipole/cut/gpu command

18.136 pair_style lj/cut/dipole/cut/omp command

18.137 pair_style lj/sf/dipole/sf command

18.138 pair_style lj/sf/dipole/sf/gpu command

18.139 pair_style lj/sf/dipole/sf/omp command

18.140 pair_style lj/cut/dipole/long command

18.141 pair_style lj/cut/dipole/long/gpu command

18.142 pair_style lj/long/dipole/long command

18.142.1 Syntax

```
pair_style lj/cut/dipole/cut cutoff (cutoff2)
pair_style lj/sf/dipole/sf cutoff (cutoff2)
pair_style lj/cut/dipole/long cutoff (cutoff2)
pair_style lj/long/dipole/long flag_lj flag_coul cutoff (cutoff2)
```

- cutoff = global cutoff LJ (and Coulombic if only 1 arg) (distance units)
- cutoff2 = global cutoff for Coulombic and dipole (optional) (distance units)
- flag_lj = *long* or *cut* or *off*

```
long = use long-range damping on dispersion 1/r^6 term
cut = use a cutoff on dispersion 1/r^6 term
off = omit disperion 1/r^6 term entirely
```

- flag_coul = *long* or *off*

```
long = use long-range damping on Coulombic 1/r and point-dipole terms
off = omit Coulombic and point-dipole terms entirely
```

18.142.2 Examples

```
pair_style lj/cut/dipole/cut 10.0
pair_coeff * * 1.0 1.0
pair_coeff 2 3 1.0 1.0 2.5 4.0

pair_style lj/sf/dipole/sf 9.0
pair_coeff * * 1.0 1.0
pair_coeff 2 3 1.0 1.0 2.5 4.0 scale 0.5
pair_coeff 2 3 1.0 1.0 2.5 4.0

pair_style lj/cut/dipole/long 10.0
pair_coeff * * 1.0 1.0
pair_coeff 2 3 1.0 1.0 2.5 4.0

pair_style lj/long/dipole/long long long 3.5 10.0
pair_coeff * * 1.0 1.0
pair_coeff 2 3 1.0 1.0 2.5 4.0
```

18.142.3 Description

Style *lj/cut/dipole/cut* computes interactions between pairs of particles that each have a charge and/or a point dipole moment. In addition to the usual Lennard-Jones interaction between the particles (Elj) the charge-charge (Eqq), charge-dipole (Eqp), and dipole-dipole (Epp) interactions are computed by these formulas for the energy (E), force

(F), and torque (T) between particles I and J.

$$
\begin{aligned}
E_{LJ} =& 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \\
E_{qq} =& \frac{q_i q_j}{r} \\
E_{qp} =& \frac{q}{r^3} (p \bullet \vec{r}) \\
E_{pp} =& \frac{1}{r^3} (\vec{p_i} \bullet \vec{p_j}) - \frac{3}{r^5} (\vec{p_i} \bullet \vec{r})(\vec{p_j} \bullet \vec{r})
\end{aligned}
$$

$$
\begin{aligned}
F_{qq} =& \frac{q_i q_j}{r^3} \vec{r} \\
F_{qp} =& -\frac{q}{r^3} \vec{p} + \frac{3q}{r^5} (\vec{p} \bullet \vec{r}) \vec{r} \\
F_{pp} =& \frac{3}{r^5} (\vec{p_i} \bullet \vec{p_j}) \vec{r} - \frac{15}{r^7} (\vec{p_i} \bullet \vec{r})(\vec{p_j} \bullet \vec{r}) \vec{r} + \frac{3}{r^5} \left[(\vec{p_j} \bullet \vec{r}) \vec{p_i} + (\vec{p_i} \bullet \vec{r}) \vec{p_j} \right]
\end{aligned}
$$

$$
\begin{aligned}
T_{pq} = T_{ij} =& \frac{q_j}{r^3} (\vec{p_i} \times \vec{r}) \\
T_{qp} = T_{ji} =& -\frac{q_i}{r^3} (\vec{p_j} \times \vec{r}) \\
T_{pp} = T_{ij} =& -\frac{1}{r^3} (\vec{p_i} \times \vec{p_j}) + \frac{3}{r^5} (\vec{p_j} \bullet \vec{r})(\vec{p_i} \times \vec{r}) \\
T_{pp} = T_{ji} =& -\frac{1}{r^3} (\vec{p_j} \times \vec{p_i}) + \frac{3}{r^5} (\vec{p_i} \bullet \vec{r})(\vec{p_j} \times \vec{r})
\end{aligned}
$$

where q_i and q_j are the charges on the two particles, $\vec{p_i}$ and $\vec{p_j}$ are the dipole moment vectors of the two particles, r is their separation distance, and the vector r = Ri - Rj is the separation vector between the two particles. Note that Eqq and Fqq are simply Coulombic energy and force, Fij = -Fji as symmetric forces, and Tij != -Tji since the torques do not act symmetrically. These formulas are discussed in *(Allen)* and in *(Toukmaji)*.

Also note, that in the code, all of these terms (except Elj) have a C/ϵ prefactor, the same as the Coulombic term in the LJ + Coulombic pair styles discussed *here*. C is an energy-conversion constant and epsilon is the dielectric constant which can be set by the *dielectric* command. The same is true of the equations that follow for other dipole pair styles.

Style *lj/sf/dipole/sf* computes "shifted-force" interactions between pairs of particles that each have a charge and/or a point dipole moment. In general, a shifted-force potential is a (slightly) modified potential containing extra terms that make both the energy and its derivative go to zero at the cutoff distance; this removes (cutoff-related) problems in energy conservation and any numerical instability in the equations of motion *(Allen)*. Shifted-force interactions for the Lennard-Jones (E_LJ), charge-charge (Eqq), charge-dipole (Eqp), dipole-charge (Epq) and dipole-dipole (Epp)

potentials are computed by these formulas for the energy (E), force (F), and torque (T) between particles I and J:

$$
\begin{aligned}
E_{LJ} =& 4\epsilon \left\{ \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] + \left[6\left(\frac{\sigma}{r_c}\right)^{12} - 3\left(\frac{\sigma}{r_c}\right)^{6} \right] \left(\frac{r}{r_c}\right)^{2} - 7\left(\frac{\sigma}{r_c}\right)^{12} + 4\left(\frac{\sigma}{r_c}\right)^{6} \right\} \\
E_{qq} =& \frac{q_i q_j}{r} \left(1 - \frac{r}{r_c}\right)^{2} \\
E_{pq} =& E_{ji} = -\frac{q}{r^3} \left[1 - 3\left(\frac{r}{r_c}\right)^{2} + 2\left(\frac{r}{r_c}\right)^{3} \right] (\vec{p} \bullet \vec{r}) \\
E_{qp} =& E_{ij} = \frac{q}{r^3} \left[1 - 3\left(\frac{r}{r_c}\right)^{2} + 2\left(\frac{r}{r_c}\right)^{3} \right] (\vec{p} \bullet \vec{r}) \\
E_{pp} =& \left[1 - 4\left(\frac{r}{r_c}\right)^{3} + 3\left(\frac{r}{r_c}\right)^{4} \right] \left[\frac{1}{r^3}(\vec{p_i} \bullet \vec{p_j}) - \frac{3}{r^5}(\vec{p_i} \bullet \vec{r})(\vec{p_j} \bullet \vec{r}) \right]
\end{aligned}
$$

$$
\begin{aligned}
F_{LJ} =& \left\{ \left[48\epsilon \left(\frac{\sigma}{r}\right)^{12} - 24\epsilon \left(\frac{\sigma}{r}\right)^{6} \right] \frac{1}{r^2} - \left[48\epsilon \left(\frac{\sigma}{r_c}\right)^{12} - 24\epsilon \left(\frac{\sigma}{r_c}\right)^{6} \right] \frac{1}{r_c^2} \right\} \vec{r} \\
F_{qq} =& \frac{q_i q_j}{r} \left(\frac{1}{r^2} - \frac{1}{r_c^2} \right) \vec{r} \\
F_{pq} =& F_{ij} = -\frac{3q}{r^5} \left[1 - \left(\frac{r}{r_c}\right)^{2} \right] (\vec{p} \bullet \vec{r})\vec{r} + \frac{q}{r^3} \left[1 - 3\left(\frac{r}{r_c}\right)^{2} + 2\left(\frac{r}{r_c}\right)^{3} \right] \vec{p} \\
F_{qp} =& F_{ij} = \frac{3q}{r^5} \left[1 - \left(\frac{r}{r_c}\right)^{2} \right] (\vec{p} \bullet \vec{r})\vec{r} - \frac{q}{r^3} \left[1 - 3\left(\frac{r}{r_c}\right)^{2} + 2\left(\frac{r}{r_c}\right)^{3} \right] \vec{p} \\
F_{pp} =& \frac{3}{r^5} \left\{ \left[1 - \left(\frac{r}{r_c}\right)^{4} \right] \left[(\vec{p_i} \bullet \vec{p_j}) - \frac{3}{r^2}(\vec{p_i} \bullet \vec{r})(\vec{p_j} \bullet \vec{r}) \right] \vec{r} + \right. \\
& \left. \left[1 - 4\left(\frac{r}{r_c}\right)^{3} + 3\left(\frac{r}{r_c}\right)^{4} \right] \left[(\vec{p_j} \bullet \vec{r})\vec{p_i} + (\vec{p_i} \bullet \vec{r})\vec{p_j} - \frac{2}{r^2}(\vec{p_i} \bullet \vec{r})(\vec{p_j} \bullet \vec{r})\vec{r} \right] \right\}
\end{aligned}
$$

$$
\begin{aligned}
T_{pq} = T_{ij} =& \frac{q_j}{r^3} \left[1 - 3\left(\frac{r}{r_c}\right)^{2} + 2\left(\frac{r}{r_c}\right)^{3} \right] (\vec{p_i} \times \vec{r}) \\
T_{qp} = T_{ji} =& -\frac{q_i}{r^3} \left[1 - 3\left(\frac{r}{r_c}\right)^{2} + 2\left(\frac{r}{r_c}\right)^{3} \right] (\vec{p_j} \times \vec{r}) \\
T_{pp} = T_{ij} =& -\frac{1}{r^3} \left[1 - 4\left(\frac{r}{r_c}\right)^{3} + e3\left(\frac{r}{r_c}\right)^{4} \right] (\vec{p_i} \times \vec{p_j}) + \\
& \frac{3}{r^5} \left[1 - 4\left(\frac{r}{r_c}\right)^{3} + 3\left(\frac{r}{r_c}\right)^{4} \right] (\vec{p_j} \bullet \vec{r})(\vec{p_i} \times \vec{r}) \\
T_{pp} = T_{ji} =& -\frac{1}{r^3} \left[1 - 4\left(\frac{r}{r_c}\right)^{3} + 3\left(\frac{r}{r_c}\right)^{4} \right] (\vec{p_j} \times \vec{p_i}) + \\
& \frac{3}{r^5} \left[1 - 4\left(\frac{r}{r_c}\right)^{3} + 3\left(\frac{r}{r_c}\right)^{4} \right] (\vec{p_i} \bullet \vec{r})(\vec{p_j} \times \vec{r})
\end{aligned}
$$

where ϵ and σ are the standard LJ parameters, r_c is the cutoff, q_i and q_j are the charges on the two particles, $\vec{p_i}$ and $\vec{p_j}$ are the dipole moment vectors of the two particles, r is their separation distance, and the vector r = Ri - Rj is the

separation vector between the two particles. Note that Eqq and Fqq are simply Coulombic energy and force, Fij = -Fji as symmetric forces, and Tij != -Tji since the torques do not act symmetrically. The shifted-force formula for the Lennard-Jones potential is reported in *(Stoddard)*. The original (non-shifted) formulas for the electrostatic potentials, forces and torques can be found in *(Price)*. The shifted-force electrostatic potentials have been obtained by applying equation 5.13 of *(Allen)*. The formulas for the corresponding forces and torques have been obtained by applying the 'chain rule' as in appendix C.3 of *(Allen)*.

If one cutoff is specified in the pair_style command, it is used for both the LJ and Coulombic (q,p) terms. If two cutoffs are specified, they are used as cutoffs for the LJ and Coulombic (q,p) terms respectively. This pair style also supports an optional *scale* keyword as part of a pair_coeff statement, where the interactions can be scaled according to this factor. This scale factor is also made available for use with fix adapt.

Style *lj/cut/dipole/long* computes long-range point-dipole interactions as discussed in *(Toukmaji)*. Dipole-dipole, dipole-charge, and charge-charge interactions are all supported, along with the standard 12/6 Lennard-Jones interactions, which are computed with a cutoff. A *kspace_style* must be defined to use this pair style. Currently, only *kspace_style ewald/disp* support long-range point-dipole interactions.

Style *lj/long/dipole/long* also computes point-dipole interactions as discussed in *(Toukmaji)*. Long-range dipole-dipole, dipole-charge, and charge-charge interactions are all supported, along with the standard 12/6 Lennard-Jones interactions. LJ interactions can be cutoff or long-ranged.

For style *lj/long/dipole/long*, if *flag_lj* is set to *long*, no cutoff is used on the LJ 1/r^6 dispersion term. The long-range portion is calculated by using the *kspace_style ewald_disp* command. The specified LJ cutoff then determines which portion of the LJ interactions are computed directly by the pair potential versus which part is computed in reciprocal space via the Kspace style. If *flag_lj* is set to *cut*, the LJ interactions are simply cutoff, as with *pair_style lj/cut*. If *flag_lj* is set to *off*, LJ interactions are not computed at all.

If *flag_coul* is set to *long*, no cutoff is used on the Coulombic or dipole interactions. The long-range portion is calculated by using *ewald_disp* of the *kspace_style* command. If *flag_coul* is set to *off*, Coulombic and dipole interactions are not computed at all.

Atoms with dipole moments should be integrated using the *fix nve/sphere update dipole* or the *fix nvt/sphere update dipole* command to rotate the dipole moments. The *omega* option on the *fix langevin* command can be used to thermostat the rotational motion. The *compute temp/sphere* command can be used to monitor the temperature, since it includes rotational degrees of freedom. The *atom_style hybrid dipole sphere* command should be used since it defines the point dipoles and their rotational state. The magnitude and orientation of the dipole moment for each particle can be defined by the *set* command or in the "Atoms" section of the data file read in by the *read_data* command.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- ϵ (energy units)
- σ (distance units)
- cutoff1 (distance units)
- cutoff2 (distance units)

The latter 2 coefficients are optional. If not specified, the global LJ and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both LJ and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the LJ and Coulombic cutoffs for this type pair.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distances for this pair style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

For atom type pairs I,J and I != J, the A, sigma, d1, and d2 coefficients and cutoff distance for this pair style can be mixed. A is an energy value mixed like a LJ epsilon. D1 and d2 are distance values and are mixed like sigma. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style does not support the *pair_modify* shift option for the energy of the Lennard-Jones portion of the pair interaction; such energy goes to zero at the cutoff by construction.

The *pair_modify* table option is not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.142.4 Restrictions

The *lj/cut/dipole/cut*, *lj/cut/dipole/long*, and *lj/long/dipole/long* styles are part of the DIPOLE package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

The *lj/sf/dipole/sf* style is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Using dipole pair styles with *electron units* is not currently supported.

18.142.5 Related commands

pair_coeff, *set*, *read_data*, *fix nve/sphere*, *fix nvt/sphere*

Default: none

(Allen) Allen and Tildesley, Computer Simulation of Liquids, Clarendon Press, Oxford, 1987.

(Toukmaji) Toukmaji, Sagui, Board, and Darden, J Chem Phys, 113, 10913 (2000).

(Stoddard) Stoddard and Ford, Phys Rev A, 8, 1504 (1973).

(Price) Price, Stone and Alderton, Mol Phys, 52, 987 (1984).

18.143 pair_style dpd command

18.144 pair_style dpd/gpu command

18.145 pair_style dpd/intel command

18.146 pair_style dpd/omp command

18.147 pair_style dpd/tstat command

18.148 pair_style dpd/tstat/gpu command

18.149 pair_style dpd/tstat/omp command

18.149.1 Syntax

```
pair_style dpd T cutoff seed
pair_style dpd/tstat Tstart Tstop cutoff seed
```

- T = temperature (temperature units)
- Tstart,Tstop = desired temperature at start/end of run (temperature units)
- cutoff = global cutoff for DPD interactions (distance units)
- seed = random # seed (positive integer)

18.149.2 Examples

```
pair_style dpd 1.0 2.5 34387
pair_coeff * * 3.0 1.0
pair_coeff 1 1 3.0 1.0 1.0

pair_style dpd/tstat 1.0 1.0 2.5 34387
pair_coeff * * 1.0
pair_coeff 1 1 1.0 1.0
```

18.149.3 Description

Style *dpd* computes a force field for dissipative particle dynamics (DPD) following the exposition in *(Groot)*.

Style *dpd/tstat* invokes a DPD thermostat on pairwise interactions, which is equivalent to the non-conservative portion of the DPD force field. This pair-wise thermostat can be used in conjunction with any *pair style*, and in leiu of per-particle thermostats like *fix langevin* or ensemble thermostats like Nose Hoover as implemented by *fix nvt*. To use *dpd/tstat* as a thermostat for another pair style, use the *pair_style hybrid/overlay* command to compute both the desired pair interaction and the thermostat for each pair of particles.

For style *dpd*, the force on atom I due to atom J is given as a sum of 3 terms

$$\begin{aligned}
\vec{f} =& (F^C + F^D + F^R)\hat{r_{ij}} \qquad\qquad r < r_c \\
F^C =& Aw(r) \\
F^D =& -\gamma w^2(r)(\hat{r_{ij}} \bullet \vec{v_{ij}}) \\
F^R =& \sigma w(r)\alpha(\Delta t)^{-1/2} \\
w(r) =& 1 - r/r_c
\end{aligned}$$

where F^C is a conservative force, F^D is a dissipative force, and F^R is a random force. r_{ij} is a unit vector in the direction $r_i - r_j$, $V_{ij} is the vector difference in velocities of the two atoms$: $math$:alpha` is a Gaussian random number with zero mean and unit variance, dt is the timestep size, and w(r) is a weighting factor that varies between 0 and 1. r_c is the cutoff. σ is set equal to $\sqrt{2k_BT\gamma}$, where k_B is the Boltzmann constant and T is the temperature parameter in the pair_style command.

For style *dpd/tstat*, the force on atom I due to atom J is the same as the above equation, except that the conservative Fc term is dropped. Also, during the run, T is set each timestep to a ramped value from Tstart to Tstop.

For style *dpd*, the pairwise energy associated with style *dpd* is only due to the conservative force term Fc, and is shifted to be zero at the cutoff distance Rc. The pairwise virial is calculated using all 3 terms. For style *dpd/tstat* there is no pairwise energy, but the last two terms of the formula make a contribution to the virial.

For style *dpd*, the following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- A (force units)
- γ (force/velocity units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global DPD cutoff is used. Note that sigma is set equal to sqrt(2 T gamma), where T is the temperature set by the *pair_style* command so it does not need to be specified.

For style *dpd/tstat*, the coefficients defined for each pair of atoms types via the *pair_coeff* command is the same, except that A is not included.

The GPU-accelerated versions of these styles are implemented based on the work of *(Afshar)* and *(Phillips)*.

Note: If you are modeling DPD polymer chains, you may want to use the *pair_style srp* command in conjunction with these pair styles. It is a soft segmental repulsive potential (SRP) that can prevent DPD polymer chains from crossing each other.

Note: The virial calculation for pressure when using this pair style includes all the components of force listed above, including the random force.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

These pair styles do not support the *pair_modify* shift option for the energy of the pair interaction. Note that as discussed above, the energy due to the conservative Fc term is already shifted to be 0.0 at the cutoff distance Rc.

The *pair_modify* table option is not relevant for these pair styles.

These pair style do not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

These pair styles writes their information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file. Note that the user-specified random number seed is stored in the restart file, so when a simulation is restarted, each processor will re-initialize its random number generator the same way it did initially. This means the random forces will be random, but will not be the same as they would have been if the original simulation had continued past the restart time.

These pair styles can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

The *dpd/tstat* style can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

18.149.4 Restrictions

The default frequency for rebuilding neighbor lists is every 10 steps (see the *neigh_modify* command). This may be too infrequent for style *dpd* simulations since particles move rapidly and can overlap by large amounts. If this setting yields a non-zero number of "dangerous" reneighborings (printed at the end of a simulation), you should experiment with forcing reneighboring more often and see if system energies/trajectories change.

These pair styles requires you to use the *comm_modify vel yes* command so that velocities are stored by ghost atoms.

These pair styles will not restart exactly when using the *read_restart* command, though they should provide statistically similar results. This is because the forces they compute depend on atom velocities. See the *read_restart* command for more details.

18.149.5 Related commands

pair_coeff, *fix nvt*, *fix langevin*, *pair_style srp*

Default: none

(Groot) Groot and Warren, J Chem Phys, 107, 4423-35 (1997).

(Afshar) Afshar, F. Schmid, A. Pishevar, S. Worley, Comput Phys Comm, 184, 1119-1128 (2013).

(Phillips) C. L. Phillips, J. A. Anderson, S. C. Glotzer, Comput Phys Comm, 230, 7191-7201 (2011).

18.150 pair_style dpd/fdt command

18.151 pair_style dpd/fdt/energy command

18.152 pair_style dpd/fdt/energy/kk command

18.152.1 Syntax

```
pair_style style args
```

- style = *dpd/fdt* or *dpd/fdt/energy*
- args = list of arguments for a particular style

```
dpd/fdt args = T cutoff seed
  T = temperature (temperature units)
  cutoff = global cutoff for DPD interactions (distance units)
  seed = random # seed (positive integer)
dpd/fdt/energy args = cutoff seed
  cutoff = global cutoff for DPD interactions (distance units)
  seed = random # seed (positive integer)
```

18.152.2 Examples

```
pair_style dpd/fdt 300.0 2.5 34387
pair_coeff * * 3.0 1.0 2.5

pair_style dpd/fdt/energy 2.5 34387
pair_coeff * * 3.0 1.0 0.1 2.5
```

18.152.3 Description

Styles *dpd/fdt* and *dpd/fdt/energy* compute the force for dissipative particle dynamics (DPD) simulations. The *dpd/fdt* style is used to perform DPD simulations under isothermal and isobaric conditions, while the *dpd/fdt/energy* style is used to perform DPD simulations under isoenergetic and isoenthalpic conditions (see *(Lisal)*). For DPD simulations in general, the force on atom I due to atom J is given as a sum of 3 terms

$$\begin{aligned}
\vec{f} =& (F^C + F^D + F^R)\hat{r_{ij}} \qquad r < r_c \\
F^C =& Aw(r) \\
F^D =& -\gamma w^2(r)(\hat{r_{ij}} \bullet \vec{v_{ij}}) \\
F^R =& \sigma w(r)\alpha(\Delta t)^{-1/2} \\
w(r) =& 1 - r/r_c
\end{aligned}$$

where F^C is a conservative force, F^D is a dissipative force, and F^R is a random force. r_{ij} is a unit vector in the direction $r_i - r_j$, $V_{ij} is the vector difference in velocities of the two atoms$: $math$:alpha` is a Gaussian random number with zero mean and unit variance, dt is the timestep size, and w(r) is a weighting factor that varies between 0 and 1. Rc is the cutoff. The weighting factor, ω_{ij}, varies between 0 and 1, and is chosen to have the following functional form:

$$\omega_{ij} = 1 - \frac{r_{ij}}{r_c}$$

Note that alternative definitions of the weighting function exist, but would have to be implemented as a separate pair style command.

For style *dpd/fdt*, the fluctuation-dissipation theorem defines γ to be set equal to $\sigma^2/(2T)$, where T is the set point temperature specified as a pair style parameter in the above examples. The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- A (force units)
- σ (force*time^(1/2) units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global DPD cutoff is used.

Style *dpd/fdt/energy* is used to perform DPD simulations under isoenergetic and isoenthalpic conditions. The fluctuation-dissipation theorem defines γ to be set equal to $sigma^2/(2\theta)$, where :math:theta` is the average internal temperature for the pair. The particle internal temperature is related to the particle internal energy through a mesoparticle equation of state (see *fix eos*). The differential internal conductive and mechanical energies are computed within style *dpd/fdt/energy* as:

$$
\begin{aligned}
du_i^{cond} =& \kappa_{ij}(\frac{1}{\theta_i} - \frac{1}{\theta_j})\omega_{ij}^2 + \alpha_{ij}\omega_{ij}\zeta_{ij}^q(\Delta t)^{-1/2} \\
du_i^{mech} =& -\frac{1}{2}\gamma_{ij}\omega_{ij}^2(\frac{\vec{r_{ij}}}{r_{ij}} \bullet \vec{v_{ij}})^2 - \frac{\sigma_{ij}^2}{4}(\frac{1}{m_i} + \frac{1}{m_j})\omega_{ij}^2 - \frac{1}{2}\sigma_{ij}\omega_{ij}(\frac{\vec{r_{ij}}}{r_{ij}} \bullet \vec{v_{ij}})\zeta_{ij}(\Delta t)^{-1/2}
\end{aligned}
$$

where

$$
\begin{aligned}
\alpha_{ij}^2 =& 2k_B\kappa_{ij} \\
\sigma_{ij}^2 =& 2\gamma_{ij}k_B\Theta_{ij} \\
\Theta_{ij}^{-1} =& \frac{1}{2}(\frac{1}{\theta_i} + \frac{1}{\theta_j})
\end{aligned}
$$

$\zeta_i j^q$ is a second Gaussian random number with zero mean and unit variance that is used to compute the internal conductive energy. The fluctuation-dissipation theorem defines $alpha^2$ to be set equal to :math:2k_Bkappa`, where κ is the mesoparticle thermal conductivity parameter. The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- A (force units)
- σ (force*time^(1/2) units)
- κ (energy*temperature/time units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global DPD cutoff is used.

The pairwise energy associated with styles *dpd/fdt* and *dpd/fdt/energy* is only due to the conservative force term Fc, and is shifted to be zero at the cutoff distance Rc. The pairwise virial is calculated using only the conservative term.

The forces computed through the *dpd/fdt* and *dpd/fdt/energy* styles can be integrated with the velocity-Verlet integration scheme or the Shardlow splitting integration scheme described by *(Lisal)*. In the cases when these pair styles are combined with the *fix shardlow*, these pair styles differ from the other dpd styles in that the dissipative and random forces are split from the force calculation and are not computed within the pair style. Thus, only the conservative force is computed by the pair style, while the stochastic integration of the dissipative and random forces are handled through the Shardlow splitting algorithm approach. The Shardlow splitting algorithm is advantageous, especially when performing DPD under isoenergetic conditions, as it allows significantly larger timesteps to be taken.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

18.152.4 Restrictions

These commands are part of the USER-DPD package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Pair styles *dpd/fdt* and *dpd/fdt/energy* require use of the *comm_modify vel yes* option so that velocities are stored by ghost atoms.

Pair style *dpd/fdt/energy* requires *atom_style dpd* to be used in order to properly account for the particle internal energies and temperatures.

18.152.5 Related commands

pair_coeff, *fix shardlow*

Default: none

(Lisal) M. Lisal, J.K. Brennan, J. Bonet Avalos, "Dissipative particle dynamics at isothermal, isobaric, isoenergetic, and isoenthalpic conditions using Shardlow-like splitting algorithms.", J. Chem. Phys., 135, 204105 (2011).

18.153 pair_style drip command

18.153.1 Syntax

```
pair_style hybrid/overlay drip [styles ...]
```

- styles = other styles to be overlayed with drip (optional)

18.153.2 Examples

```
pair_style hybrid/overlay drip
pair_coeff * * none
pair_coeff * * drip  C.drip  C

pair_style hybrid/overlay drip rebo
pair_coeff * * drip  C.drip     C
pair_coeff * * rebo  CH.airebo  C

pair_style hybrid/overlay drip rebo
pair_coeff * * drip  C.drip     C NULL
pair_coeff * * rebo  CH.airebo  C H
```

18.153.3 Description

Style *drip* computes the interlayer interactions of layered materials using the dihedral-angle-corrected registry-dependent (DRIP) potential as described in *(Wen)*, which is based on the *(Kolmogorov)* potential and provides an improved prediction for forces. The total potential energy of a system is

$$E = \frac{1}{2} \sum_i \sum_{j \notin \text{layer } i} \phi_{ij}$$

$$\phi_{ij} = f_c(x_r) \left[e^{-\lambda(r_{ij} - z_0)} \left[C + f(\rho_{ij}) + g(\rho_{ij}, \{\alpha_{ij}^{(m)}\}) \right] - A \left(\frac{z_0}{r_{ij}} \right)^6 \right]$$

where the r^{-6} term models the attractive London dispersion, the exponential term is designed to capture the registry effect due to overlapping *pi* bonds, and *fc* is a cutoff function.

This potential (DRIP) only provides the interlayer interactions between graphene layers. So, to perform a realistic simulation, it should be used in combination with an intralayer potential such as *REBO* and *Tersoff*. To keep the intralayer interactions unaffected, we should avoid applying DRIP to contribute energy to intralayer interactions. This can be achieved by assigning different molecular IDs to atoms in different layers, and DRIP is implemented such that only atoms with different molecular ID can interact with each other. For this purpose, *atom style* "molecular" or "full" has to be used.

On the other way around, *REBO* (*Tersoff* or any other potential used to provide the intralayer interactions) should not interfere with the interlayer interactions described by DRIP. This is typically automatically achieved using the commands provided in the *Examples* section above, since the cutoff distance for carbon-carbon interaction in the intralayer potentials (e.g. 2 Angstrom for *REBO*) is much smaller than the equilibrium layer distance of graphene layers (about 3.4 Angstrom). If you want, you can enforce this by assigning different atom types to atoms in different layers, and apply an intralayer potential to one atom type. See *pair_hybrid* for details.

The *pair_coeff* command for DRIP takes *4+N* arguments, where *N* is the number of LAMMPS atom types. The fist three arguments must be fixed to be * * *drip*, the fourth argument is the path to the DRIP parameter file, and the remaining N arguments specifying the mapping between element in the parameter file and atom types. For example, if your LAMMPS simulation has 3 atom types and you want all of them to be C, you would use the following pair_coeff command:

```
pair_coeff * * drip  C.drip  C C C
```

If a mapping value is specified as NULL, the mapping is not performed. This could be useful when DRIP is used to model part of the system where other element exists. Suppose you have a hydrocarbon system, with C of atom type 1 and H of atom type 2, you can use the following command to inform DRIP not to model H atoms:

```
pair_style hybrid/overlay drip rebo
pair_coeff * * drip  C.drip     C NULL
pair_coeff * * rebo  CH.airebo  C H
```

Note: The potential parameters developed in *(Wen)* are provided with LAMMPS (see the "potentials" directory). Besides those in *Wen*, an additional parameter "normal_cutoff", specific to the LAMMPS implementation, is used to find the three nearest neighbors of an atom to construct the normal.

Mixing, shift, table, tail correction, and restart info:

This pair style does not support the pair_modify mix, shift, table, and tail options.

This pair style does not write their information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

18.153.4 Restrictions

This pair style is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This pair potential requires the *newton* setting to be "on" for pair interactions.

The *C.drip* parameter file provided with LAMMPS (see the "potentials" directory) is parameterized for metal *units*. You can use the DRIP potential with any LAMMPS units, but you would need to create your own custom parameter file with coefficients listed in the appropriate units, if your simulation doesn't use "metal" units.

18.153.5 Related commands

pair_style lebedeva_z, *pair_style kolmogorov/crespi/z*, *pair_style kolmogorov/crespi/full*, *pair_style ilp/graphene/hbn*.

(Wen) M. Wen, S. Carr, S. Fang, E. Kaxiras, and E. B. Tadmor, Phys. Rev. B, 98, 235404 (2018)

(Kolmogorov) A. N. Kolmogorov, V. H. Crespi, Phys. Rev. B 71, 235415 (2005)

18.154 pair_style dsmc command

18.154.1 Syntax

```
pair_style dsmc max_cell_size seed weighting Tref Nrecompute Nsample
```

- max_cell_size = global maximum cell size for DSMC interactions (distance units)
- seed = random # seed (positive integer)
- weighting = macroparticle weighting
- Tref = reference temperature (temperature units)
- Nrecompute = re-compute v*sigma_max every this many timesteps (timesteps)
- Nsample = sample this many times in recomputing v*sigma_max

18.154.2 Examples

```
pair_style dsmc 2.5 34387 10 1.0 100 20
pair_coeff * * 1.0
pair_coeff 1 1 1.0
```

18.154.3 Description

Style *dsmc* computes collisions between pairs of particles for a direct simulation Monte Carlo (DSMC) model following the exposition in *(Bird)*. Each collision resets the velocities of the two particles involved. The number of pairwise collisions for each pair or particle types and the length scale within which they occur are determined by the parameters of the pair_style and pair_coeff commands.

Stochastic collisions are performed using the variable hard sphere (VHS) approach, with the user-defined *max_cell_size* value used as the maximum DSMC cell size, and reference cross-sections for collisions given using the pair_coeff command.

There is no pairwise energy or virial contributions associated with this pair style.

The following coefficient must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- sigma (area units, i.e. distance-squared)

The global DSMC *max_cell_size* determines the maximum cell length used in the DSMC calculation. A structured mesh is overlayed on the simulation box such that an integer number of cells are created in each direction for each processor's sub-domain. Cell lengths are adjusted up to the user-specified maximum cell size.

To perform a DSMC simulation with LAMMPS, several additional options should be set in your input script, though LAMMPS does not check for these settings.

Since this pair style does not compute particle forces, you should use the "fix nve/noforce" time integration fix for the DSMC particles, e.g.

```
fix 1 all nve/noforce
```

This pair style assumes that all particles will communicated to neighboring processors every timestep as they move. This makes it possible to perform all collisions between pairs of particles that are on the same processor. To ensure this occurs, you should use these commands:

```
neighbor 0.0 bin
neigh_modify every 1 delay 0 check no
atom_modify sort 0 0.0
communicate single cutoff 0.0
```

These commands ensure that LAMMPS communicates particles to neighboring processors every timestep and that no ghost atoms are created. The output statistics for a simulation run should indicate there are no ghost particles or neighbors.

In order to get correct DSMC collision statistics, users should specify a Gaussian velocity distribution when populating the simulation domain. Note that the default velocity distribution is uniform, which will not give good DSMC collision rates. Specify "dist gaussian" when using the *velocity* command as in the following:

```
velocity all create 594.6 87287 loop geom dist gaussian
```

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This pair style does not support the *pair_modify* shift option for the energy of the pair interaction.

The *pair_modify* table option is not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file. Note that the user-specified random number seed is stored in the restart file, so when a simulation is restarted, each processor will re-initialize its random number generator the same way it did initially. This means the random forces will be random, but will not be the same as they would have been if the original simulation had continued past the restart time.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.154.4 Restrictions

This style is part of the MC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.154.5 Related commands

pair_coeff, *fix nve/noforce*, *neigh_modify*, *neighbor*, *comm_modify*

Default: none

(Bird) G. A. Bird, "Molecular Gas Dynamics and the Direct Simulation of Gas Flows" (1994).

18.155 pair_style e3b command

18.155.1 Syntax

```
pair_style e3b Otype
```

- Otype = atom type for oxygen

```
pair_coeff * * keyword
```

- one or more keyword/value pairs must be appended.
- keyword = *preset* or *Ea* or *Eb* or *Ec* or *E2* or *K3* or *K2* or *Rs* or *Rc3* or *Rc2* or *bondL* or *neigh*
- If the *preset* keyword is given, no others are needed. Otherwise, all are mandatory except for *neigh*. The *neigh* keyword is always optional.

```
preset arg = 2011 or 2015 = which set of predefined parameters to use
         2011 = use the potential parameters from (Tainter 2011)
         2015 = use the potential parameters from (Tainter 2015)
Ea arg = three-body energy for type A hydrogen bonding interactions (energy␣
↪units)
Eb arg = three-body energy for type B hydrogen bonding interactions (energy␣
↪units)
Ec arg = three-body energy for type C hydrogen bonding interactions (energy␣
↪units)
E2 arg = two-body energy correction (energy units)
K3 arg = three-body exponential constant (inverse distance units)
K2 arg = two-body exponential constant (inverse distance units)
Rc3 arg = three-body cutoff (distance units)
Rc2 arg = two-body cutoff (distance units)
Rs arg = three-body switching function cutoff (distance units)
bondL arg = intramolecular OH bond length (distance units)
neigh arg = approximate integer number of molecules within Rc3 of an oxygen␣
↪atom
```

18.155.2 Examples

```
pair_style e3b 1
pair_coeff * * Ea 35.85 Eb -240.2 Ec 449.3 E2 108269.9 K3 1.907 K2 4.872 Rc3 5.2 Rc2␣
↪5.2 Rs 5.0 bondL 0.9572

pair_style hybrid/overlay e3b 1 lj/cut/tip4p/long 1 2 1 1 0.15 8.5
pair_coeff * * e3b preset 2011
```

18.155.3 Description

The *e3b* style computes an "explicit three-body" (E3B) potential for water *(Kumar 2008)*.

$$E = E_2 \sum_{i,j} e^{-k_2 r_{ij}} + E_A \sum_{\substack{i,j,k,\ell \\ \in \text{type A}}} f(r_{ij}) f(r_{k\ell}) + E_B \sum_{\substack{i,j,k,\ell \\ \in \text{type B}}} f(r_{ij}) f(r_{k\ell}) + E_C \sum_{\substack{i,j,k,\ell \\ \in \text{type C}}} f(r_{ij}) f(r_{k\ell})$$

$$f(r) = e^{-k_3 r} s(r)$$

$$s(r) = \begin{cases} 1 & r < R_s \\ \dfrac{(R_f - r)^2 (R_f - 3R_s + 2r)}{(R_f - R_s)^3} & R_s \le r \le R_f \\ 0 & r > R_f \end{cases}$$

This potential was developed as a water model that includes the three-body cooperativity of hydrogen bonding explicitly. To use it in this way, it must be applied in conjunction with a conventional two-body water model, through *pair_style hybrid/overlay*. The three body interactions are split into three types: A, B, and C. Type A corresponds to anti-cooperative double hydrogen bond donor interactions. Type B corresponds to the cooperative interaction of molecules that both donate and accept a hydrogen bond. Type C corresponds to anti-cooperative double hydrogen bond acceptor interactions. The three-body interactions are smoothly cutoff by the switching function s(r) between Rs and Rc3. The two-body interactions are designed to correct for the effective many-body interactions implicitly included in the conventional two-body potential. The two-body interactions are cut off sharply at Rc2, because K3 is typically significantly smaller than K2. See *(Kumar 2008)* for more details.

Only a single *pair_coeff* command is used with the *e3b* style. The 1st two arguments must be * *. The oxygen atom type for the pair style is passed as the only argument to the *pair_style* command, not in the *pair_coeff* command. The hydrogen atom type is inferred by the ordering of the atoms.

Note: Every atom of type Otype must be part of a water molecule. Each water molecule must have consecutive IDs with the oxygen first. This pair style does not test that this criteria is met.

The *pair_coeff* command must have at least one keyword/value pair, as described above. The *preset* keyword sets the potential parameters to the values used in *(Tainter 2011)* or *(Tainter 2015)*. To use the water models defined in those references, the *e3b* style should always be used in conjunction with an *lj/cut/tip4p/long* style through *pair_style hybrid/overlay*, as demonstrated in the second example above. The *preset 2011* option should be used with the *TIP4P water model*. The *preset 2015* option should be used with the *TIP4P/2005 water model*. If the *preset* keyword is used, no other keyword is needed. Changes to the preset parameters can be made by specifying the *preset* keyword followed by the specific parameter to change, like *Ea*. Note that the other keywords must come after *preset* in the pair_style command. The *e3b* style can also be used to implement any three-body potential of the same form by specifying all the keywords except *neigh*: *Ea*, *Eb*, *Ec*, *E2*, *K3*, *K2*, *Rc3*, *Rc2*, *Rs*, and *bondL*. The keyword *bondL* specifies the intramolecular OH bond length of the water model being used. This is needed to include H atoms that are within the cutoff even when the attached oxygen atom is not.

This pair style allocates arrays sized according to the number of pairwise interactions within Rc3. To do this it needs an estimate for the number of water molecules within Rc3 of an oxygen atom. This estimate defaults to 10 and can be changed using the *neigh* keyword, which takes an integer as an argument. If the neigh setting is too small, the simulation will fail with the error "neigh is too small". If the neigh setting is too large, the pair style will use more memory than necessary.

This pair style tallies a breakdown of the total E3B potential energy into sub-categories, which can be accessed via the *compute pair* command as a vector of values of length 4. The 4 values correspond to the terms in the first equation above: the E2 term, the Ea term, the Eb term, and the Ec term.

See the examples/USER/misc/e3b directory for a complete example script.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style does not write its information to *binary restart files*. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style is incompatible with *respa*.

18.155.4 Restrictions

This pair style is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This pair style requires the *newton* setting to be "on" for pair interactions.

This pair style requires a fixed number of atoms in the simulation, so it is incompatible with fixes like *fix deposit*. If the number of atoms changes between runs, this pair style must be re-initialized by calling the *pair_style* and *pair_coeffs* commands. This is not a fundamental limitation of the pair style, but the code currently does not support a variable number of atoms.

The *preset* keyword currently only works with real, metal, si, and cgs *units*.

18.155.5 Related commands

pair_coeff, *compute pair*

18.155.6 Default

The option default for the *neigh* keyword is 10.

(Kumar) Kumar and Skinner, J. Phys. Chem. B, 112, 8311 (2008)

(Tainter 2011) Tainter, Pieniazek, Lin, and Skinner, J. Chem. Phys., 134, 184501 (2011)

(Tainter 2015) Tainter, Shi, and Skinner, 11, 2268 (2015)

18.156 pair_style eam command

18.157 pair_style eam/gpu command

18.158 pair_style eam/intel command

18.159 pair_style eam/kk command

18.160 pair_style eam/omp command

18.161 pair_style eam/opt command

18.162 pair_style eam/alloy command

18.163 pair_style eam/alloy/gpu command

18.164 pair_style eam/alloy/intel command

18.165 pair_style eam/alloy/kk command

18.166 pair_style eam/alloy/omp command

18.167 pair_style eam/alloy/opt command

18.168 pair_style eam/cd command

18.169 pair_style eam/cd/omp command

18.170 pair_style eam/cd/old command

18.171 pair_style eam/cd/old/omp command

18.172 pair_style eam/fs command

18.173 pair_style eam/fs/gpu command

18.174 pair_style eam/fs/intel command

18.175 pair_style eam/fs/kk command

18.176 pair_style eam/fs/omp command

18.177 pair_style eam/fs/opt command

```
pair_style style
```

- style = *eam* or *eam/alloy* or *eam/cd* or *eam/cd/old* or *eam/fs*

18.177.2 Examples

```
pair_style eam
pair_coeff * * cuu3
pair_coeff 1*3 1\*3 niu3.eam

pair_style eam/alloy
pair_coeff * * ../potentials/NiAlH_jea.eam.alloy Ni Al Ni Ni

pair_style eam/cd
pair_coeff * * ../potentials/FeCr.cdeam Fe Cr

pair_style eam/fs
pair_coeff * * NiAlH_jea.eam.fs Ni Al Ni Ni
```

18.177.3 Description

Style *eam* computes pairwise interactions for metals and metal alloys using embedded-atom method (EAM) potentials *(Daw)*. The total energy Ei of an atom I is given by

$$E_i = F_\alpha \left(\sum_{j \neq i} \rho_\beta(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij})$$

where F is the embedding energy which is a function of the atomic electron density rho, phi is a pair potential interaction, and alpha and beta are the element types of atoms I and J. The multi-body nature of the EAM potential is a result of the embedding energy term. Both summations in the formula are over all neighbors J of atom I within the cutoff distance.

The cutoff distance and the tabulated values of the functionals F, rho, and phi are listed in one or more files which are specified by the *pair_coeff* command. These are ASCII text files in a DYNAMO-style format which is described below. DYNAMO was the original serial EAM MD code, written by the EAM originators. Several DYNAMO potential files for different metals are included in the "potentials" directory of the LAMMPS distribution. All of these files are parameterized in terms of LAMMPS *metal units*.

Note: The *eam* style reads single-element EAM potentials in the DYNAMO *funcfl* format. Either single element or alloy systems can be modeled using multiple *funcfl* files and style *eam*. For the alloy case LAMMPS mixes the single-element potentials to produce alloy potentials, the same way that DYNAMO does. Alternatively, a single DYNAMO *setfl* file or Finnis/Sinclair EAM file can be used by LAMMPS to model alloy systems by invoking the *eam/alloy* or *eam/cd* or *eam/fs* styles as described below. These files require no mixing since they specify alloy interactions explicitly.

Note: Note that unlike for other potentials, cutoffs for EAM potentials are not set in the pair_style or pair_coeff command; they are specified in the EAM potential files themselves. Likewise, the EAM potential files list atomic masses; thus you do not need to use the *mass* command to specify them.

There are several WWW sites that distribute and document EAM potentials stored in DYNAMO or other formats:

```
http://www.ctcms.nist.gov/potentials
http://cst-www.nrl.navy.mil/ccm6/ap
http://enpub.fulton.asu.edu/cms/potentials/main/main.htm
```

These potentials should be usable with LAMMPS, though the alternate formats would need to be converted to the DYNAMO format used by LAMMPS and described on this page. The NIST site is maintained by Chandler Becker (cbecker at nist.gov) who is good resource for info on interatomic potentials and file formats.

For style *eam*, potential values are read from a file that is in the DYNAMO single-element *funcfl* format. If the DYNAMO file was created by a Fortran program, it cannot have "D" values in it for exponents. C only recognizes "e" or "E" for scientific notation.

Note that unlike for other potentials, cutoffs for EAM potentials are not set in the pair_style or pair_coeff command; they are specified in the EAM potential files themselves.

For style *eam* a potential file must be assigned to each I,I pair of atom types by using one or more pair_coeff commands, each with a single argument:

- filename

Thus the following command

```
pair_coeff *2 1*2 cuu3.eam
```

will read the cuu3 potential file and use the tabulated Cu values for F, phi, rho that it contains for type pairs 1,1 and 2,2 (type pairs 1,2 and 2,1 are ignored). See the *pair_coeff* doc page for alternate ways to specify the path for the potential file. In effect, this makes atom types 1 and 2 in LAMMPS be Cu atoms. Different single-element files can be assigned to different atom types to model an alloy system. The mixing to create alloy potentials for type pairs with I != J is done automatically the same way that the serial DYNAMO code originally did it; you do not need to specify coefficients for these type pairs.

Funcfl files in the *potentials* directory of the LAMMPS distribution have an ".eam" suffix. A DYNAMO single-element *funcfl* file is formatted as follows:

- line 1: comment (ignored)
- line 2: atomic number, mass, lattice constant, lattice type (e.g. FCC)
- line 3: Nrho, drho, Nr, dr, cutoff

On line 2, all values but the mass are ignored by LAMMPS. The mass is in mass *units*, e.g. mass number or grams/mole for metal units. The cubic lattice constant is in Angstroms. On line 3, Nrho and Nr are the number of tabulated values in the subsequent arrays, drho and dr are the spacing in density and distance space for the values in those arrays, and the specified cutoff becomes the pairwise cutoff used by LAMMPS for the potential. The units of dr are Angstroms; I'm not sure of the units for drho - some measure of electron density.

Following the three header lines are three arrays of tabulated values:

- embedding function F(rho) (Nrho values)
- effective charge function Z(r) (Nr values)
- density function rho(r) (Nr values)

The values for each array can be listed as multiple values per line, so long as each array starts on a new line. For example, the individual Z(r) values are for r = 0,dr,2*dr, ... (Nr-1)*dr.

The units for the embedding function F are eV. The units for the density function rho are the same as for drho (see above, electron density). The units for the effective charge Z are "atomic charge" or sqrt(Hartree * Bohr-radii). For

two interacting atoms i,j this is used by LAMMPS to compute the pair potential term in the EAM energy expression as r*phi, in units of eV-Angstroms, via the formula

$$r \cdot \phi = 27.2 \cdot 0.529 \cdot Z_i \cdot Z_j$$

where 1 Hartree = 27.2 eV and 1 Bohr = 0.529 Angstroms.

Style *eam/alloy* computes pairwise interactions using the same formula as style *eam*. However the associated *pair_coeff* command reads a DYNAMO *setfl* file instead of a *funcfl* file. *Setfl* files can be used to model a single-element or alloy system. In the alloy case, as explained above, *setfl* files contain explicit tabulated values for alloy interactions. Thus they allow more generality than *funcfl* files for modeling alloys.

For style *eam/alloy*, potential values are read from a file that is in the DYNAMO multi-element *setfl* format, except that element names (Ni, Cu, etc) are added to one of the lines in the file. If the DYNAMO file was created by a Fortran program, it cannot have "D" values in it for exponents. C only recognizes "e" or "E" for scientific notation.

Only a single pair_coeff command is used with the *eam/alloy* style which specifies a DYNAMO *setfl* file, which contains information for M elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of *setfl* elements to atom types

As an example, the potentials/NiAlH_jea.eam.alloy file is a *setfl* file which has tabulated EAM values for 3 elements and their alloy interactions: Ni, Al, and H. See the *pair_coeff* doc page for alternate ways to specify the path for the potential file. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Ni, and the 4th to be Al, you would use the following pair_coeff command:

```
pair_coeff * * NiAlH_jea.eam.alloy Ni Ni Ni Al
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Ni arguments map LAMMPS atom types 1,2,3 to the Ni element in the *setfl* file. The final Al argument maps LAMMPS atom type 4 to the Al element in the *setfl* file. Note that there is no requirement that your simulation use all the elements specified by the *setfl* file.

If a mapping value is specified as NULL, the mapping is not performed. This can be used when an *eam/alloy* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Setfl files in the *potentials* directory of the LAMMPS distribution have an ".eam.alloy" suffix. A DYNAMO multi-element *setfl* file is formatted as follows:

- lines 1,2,3 = comments (ignored)
- line 4: Nelements Element1 Element2 ... ElementN
- line 5: Nrho, drho, Nr, dr, cutoff

In a DYNAMO *setfl* file, line 4 only lists Nelements = the # of elements in the *setfl* file. For LAMMPS, the element name (Ni, Cu, etc) of each element must be added to the line, in the order the elements appear in the file.

The meaning and units of the values in line 5 is the same as for the *funcfl* file described above. Note that the cutoff (in Angstroms) is a global value, valid for all pairwise interactions for all element pairings.

Following the 5 header lines are Nelements sections, one for each element, each with the following format:

- line 1 = atomic number, mass, lattice constant, lattice type (e.g. FCC)
- embedding function F(rho) (Nrho values)

- density function rho(r) (Nr values)

As with the *funcfl* files, only the mass (in mass *units*, e.g. mass number or grams/mole for metal units) is used by LAMMPS from the 1st line. The cubic lattice constant is in Angstroms. The F and rho arrays are unique to a single element and have the same format and units as in a *funcfl* file.

Following the Nelements sections, Nr values for each pair potential phi(r) array are listed for all i,j element pairs in the same format as other arrays. Since these interactions are symmetric (i,j = j,i) only phi arrays with i >= j are listed, in the following order: i,j = (1,1), (2,1), (2,2), (3,1), (3,2), (3,3), (4,1), . . . , (Nelements, Nelements). Unlike the effective charge array Z(r) in *funcfl* files, the tabulated values for each phi function are listed in *setfl* files directly as r*phi (in units of eV-Angstroms), since they are for atom pairs.

Style *eam/cd* is similar to the *eam/alloy* style, except that it computes alloy pairwise interactions using the concentration-dependent embedded-atom method (CD-EAM). This model can reproduce the enthalpy of mixing of alloys over the full composition range, as described in *(Stukowski)*. Style *eam/cd/old* is an older, slightly different and slower two-site formulation of the model *(Caro)*.

The pair_coeff command is specified the same as for the *eam/alloy* style. However the DYNAMO *setfl* file must has two lines added to it, at the end of the file:

- line 1: Comment line (ignored)
- line 2: N Coefficient0 Coefficient1 . . . CoefficientN

The last line begins with the degree *N* of the polynomial function *h(x)* that modifies the cross interaction between A and B elements. Then *N+1* coefficients for the terms of the polynomial are then listed.

Modified EAM *setfl* files used with the *eam/cd* style must contain exactly two elements, i.e. in the current implementation the *eam/cd* style only supports binary alloys. The first and second elements in the input EAM file are always taken as the *A* and *B* species.

CD-EAM files in the *potentials* directory of the LAMMPS distribution have a ".cdeam" suffix.

Style *eam/fs* computes pairwise interactions for metals and metal alloys using a generalized form of EAM potentials due to Finnis and Sinclair *(Finnis)*. The total energy Ei of an atom I is given by

$$E_i = F_\alpha \left(\sum_{j \neq i} \rho_{\alpha\beta}(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij})$$

This has the same form as the EAM formula above, except that rho is now a functional specific to the atomic types of both atoms I and J, so that different elements can contribute differently to the total electron density at an atomic site depending on the identity of the element at that atomic site.

The associated *pair_coeff* command for style *eam/fs* reads a DYNAMO *setfl* file that has been extended to include additional rho_alpha_beta arrays of tabulated values. A discussion of how FS EAM differs from conventional EAM alloy potentials is given in *(Ackland1)*. An example of such a potential is the same author's Fe-P FS potential *(Ackland2)*. Note that while FS potentials always specify the embedding energy with a square root dependence on the total density, the implementation in LAMMPS does not require that; the user can tabulate any functional form desired in the FS potential files.

For style *eam/fs*, the form of the pair_coeff command is exactly the same as for style *eam/alloy*, e.g.

```
pair_coeff * * NiAlH_jea.eam.fs Ni Ni Ni Al
```

where there are N additional arguments after the filename, where N is the number of LAMMPS atom types. See the *pair_coeff* doc page for alternate ways to specify the path for the potential file. The N values determine the mapping

of LAMMPS atom types to EAM elements in the file, as described above for style *eam/alloy*. As with *eam/alloy*, if a mapping value is NULL, the mapping is not performed. This can be used when an *eam/fs* potential is used as part of the *hybrid* pair style. The NULL values are used as placeholders for atom types that will be used with other potentials.

FS EAM files include more information than the DYNAMO *setfl* format files read by *eam/alloy*, in that i,j density functionals for all pairs of elements are included as needed by the Finnis/Sinclair formulation of the EAM.

FS EAM files in the *potentials* directory of the LAMMPS distribution have an ".eam.fs" suffix. They are formatted as follows:

- lines 1,2,3 = comments (ignored)
- line 4: Nelements Element1 Element2 ... ElementN
- line 5: Nrho, drho, Nr, dr, cutoff

The 5-line header section is identical to an EAM *setfl* file.

Following the header are Nelements sections, one for each element I, each with the following format:

- line 1 = atomic number, mass, lattice constant, lattice type (e.g. FCC)
- embedding function F(rho) (Nrho values)
- density function rho(r) for element I at element 1 (Nr values)
- density function rho(r) for element I at element 2
- ...
- density function rho(r) for element I at element Nelement

The units of these quantities in line 1 are the same as for *setfl* files. Note that the rho(r) arrays in Finnis/Sinclair can be asymmetric (i,j != j,i) so there are Nelements^2 of them listed in the file.

Following the Nelements sections, Nr values for each pair potential phi(r) array are listed in the same manner (r*phi, units of eV-Angstroms) as in EAM *setfl* files. Note that in Finnis/Sinclair, the phi(r) arrays are still symmetric, so only phi arrays for i >= j are listed.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above with the individual styles. You never need to specify a pair_coeff command with I != J arguments for the eam styles.

This pair style does not support the *pair_modify* shift, table, and tail options.

The eam pair styles do not write their information to *binary restart files*, since it is stored in tabulated potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

The eam pair styles can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

18.177.4 Restrictions

All of these styles are part of the MANYBODY package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.177.5 Related commands

pair_coeff

Default: none

(Ackland1) Ackland, Condensed Matter (2005).

(Ackland2) Ackland, Mendelev, Srolovitz, Han and Barashev, Journal of Physics: Condensed Matter, 16, S2629 (2004).

(Daw) Daw, Baskes, Phys Rev Lett, 50, 1285 (1983). Daw, Baskes, Phys Rev B, 29, 6443 (1984).

(Finnis) Finnis, Sinclair, Philosophical Magazine A, 50, 45 (1984).

(Stukowski) Stukowski, Sadigh, Erhart, Caro; Modeling Simulation Materials Science & Engineering, 7, 075005 (2009).

(Caro) A Caro, DA Crowson, M Caro; Phys Rev Lett, 95, 075702 (2005)

18.178 pair_style edip command

18.179 pair_style edip/omp command

18.180 pair_style edip/multi command

18.180.1 Syntax

```
pair_style style
```

- style = *edip* or *edip/multi*

18.180.2 Examples

```
pair_style edip
pair_coeff * * Si.edip Si
```

18.180.3 Description

The *edip* and *edip/multi* styles compute a 3-body *EDIP* potential which is popular for modeling silicon materials where it can have advantages over other models such as the *Stillinger-Weber* or *Tersoff* potentials. The *edip* style has been programmed for single element potentials, while *edip/multi* supports multi-element EDIP runs.

In EDIP, the energy E of a system of atoms is

$$
\begin{aligned}
E =& \sum_{j \neq i} \phi_2(R_{ij}, Z_i) + \sum_{j \neq i} \sum_{k \neq i, k > j} \phi_3(R_{ij}, R_{ik}, Z_i) \\
\phi_2(r, Z) =& A \left[\left(\frac{B}{r} \right)^{\rho} - e^{-\beta Z^2} \right] exp\left(\frac{\sigma}{r - a} \right) \\
\phi_3(R_{ij}, R_{ik}, Z_i) =& exp\left(\frac{\gamma}{R_{ij} - a} \right) exp\left(\frac{\gamma}{R_{ik} - a} \right) h(cos\theta_{ijk}, Z_i) \\
Z_i =& \sum_{m \neq i} f(R_{im}) \qquad f(r) = \begin{cases} 1 & r < c \\ \exp\left(\frac{\alpha}{1 - x^{-3}} \right) & c < r < a \\ 0 & r > a \end{cases} \\
h(l, Z) =& \lambda[(1 - e^{-Q(Z)(l + \tau(Z))^2}) + \eta Q(Z)(l + \tau(Z))^2] \\
Q(Z) =& Q_0 e^{-\mu Z} \qquad \tau(Z) = u_1 + u_2(u_3 e^{-u_4 Z} - e^{-2u_4 Z})
\end{aligned}
$$

where ϕ_2 is a two-body term and ϕ_3 is a three-body term. The summations in the formula are over all neighbors J and K of atom I within a cutoff distance = a. Both terms depend on the local environment of atom I through its effective coordination number defined by Z, which is unity for a cutoff distance < c and gently goes to 0 at distance = a.

Only a single pair_coeff command is used with the *edip* style which specifies a EDIP potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of EDIP elements to atom types

See the *pair_coeff* doc page for alternate ways to specify the path for the potential file.

As an example, imagine a file Si.edip has EDIP values for Si.

EDIP files in the *potentials* directory of the LAMMPS distribution have a ".edip" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements. The parameters in a single entry correspond to the two-body and three-body coefficients in the formula above:

- element 1 (the center atom in a 3-body interaction)
- element 2
- element 3
- A (energy units)
- B (distance units)
- cutoffA (distance units)

- cutoffC (distance units)
- α
- β
- η
- γ (distance units)
- $lambda$ (energy units)
- μ
- τ
- σ (distance units)
- Q0
- u1
- u2
- u3
- u4

The A, B, beta, sigma parameters are used only for two-body interactions. The eta, gamma, lambda, mu, Q0 and all u1 to u4 parameters are used only for three-body interactions. The alpha and cutoffC parameters are used for the coordination environment function only.

The EDIP potential file must contain entries for all the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries.

For a single-element simulation, only a single entry is required (e.g. SiSiSi). For a two-element simulation, the file must contain 8 entries (for SiSiSi, SiSiC, SiCSi, SiCC, CSiSi, CSiC, CCSi, CCC), that specify EDIP parameters for all permutations of the two elements interacting in three-body configurations. Thus for 3 elements, 27 entries would be required, etc.

At the moment, only a single element parameterization is implemented. However, the author is not aware of other multi-element EDIP parameterization. If you know any and you are interest in that, please contact the author of the EDIP package.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.180.4 Restrictions

This pair style can only be used if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

This pair style requires the *newton* setting to be "on" for pair interactions.

The EDIP potential files provided with LAMMPS (see the potentials directory) are parameterized for metal *units*. You can use the EDIP potential with any LAMMPS units, but you would need to create your own EDIP potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

18.180.5 Related commands

pair_coeff

Default: none

(EDIP) J F Justo et al, Phys Rev B 58, 2539 (1998).

18.181 pair_style eff/cut command

18.181.1 Syntax

```
pair_style eff/cut cutoff keyword args ...
```

- cutoff = global cutoff for Coulombic interactions
- zero or more keyword/value pairs may be appended

```
keyword = limit/eradius or pressure/evirials or ecp
  limit/eradius args = none
  pressure/evirials args = none
  ecp args = type element type element ...
    type = LAMMPS atom type (1 to Ntypes)
    element = element symbol (e.g. H, Si)
```

18.181.2 Examples

```
pair_style eff/cut 39.7
pair_style eff/cut 40.0 limit/eradius
pair_style eff/cut 40.0 limit/eradius pressure/evirials
pair_style eff/cut 40.0 ecp 1 Si 3 C
pair_coeff * *
pair_coeff 2 2 20.0
pair_coeff 1 s 0.320852 2.283269 0.814857
pair_coeff 3 p 22.721015 0.728733 1.103199 17.695345 6.693621
```

18.181.3 Description

This pair style contains a LAMMPS implementation of the electron Force Field (eFF) potential currently under development at Caltech, as described in *(Jaramillo-Botero)*. The eFF for Z<6 was first introduced by *(Su)* in 2007. It has been extended to higher Zs by using effective core potentials (ECPs) that now cover up to 2nd and 3rd row p-block elements of the periodic table.

eFF can be viewed as an approximation to QM wave packet dynamics and Fermionic molecular dynamics, combining the ability of electronic structure methods to describe atomic structure, bonding, and chemistry in materials, and of plasma methods to describe nonequilibrium dynamics of large systems with a large number of highly excited electrons. Yet, eFF relies on a simplification of the electronic wave function in which electrons are described as floating Gaussian wave packets whose position and size respond to the various dynamic forces between interacting classical nuclear particles and spherical Gaussian electron wave packets. The wave function is taken to be a Hartree product of the wave packets. To compensate for the lack of explicit antisymmetry in the resulting wave function, a spin-dependent Pauli potential is included in the Hamiltonian. Substituting this wave function into the time-dependent Schrodinger equation produces equations of motion that correspond - to second order - to classical Hamiltonian relations between electron position and size, and their conjugate momenta. The N-electron wave function is described as a product of one-electron Gaussian functions, whose size is a dynamical variable and whose position is not constrained to a nuclear center. This form allows for straightforward propagation of the wave function, with time, using a simple formulation from which the equations of motion are then integrated with conventional MD algorithms. In addition to this spin-dependent Pauli repulsion potential term between Gaussians, eFF includes the electron kinetic energy from the Gaussians. These two terms are based on first-principles quantum mechanics. On the other hand, nuclei are described as point charges, which interact with other nuclei and electrons through standard electrostatic potential forms.

The full Hamiltonian (shown below), contains then a standard description for electrostatic interactions between a set of delocalized point and Gaussian charges which include, nuclei-nuclei (NN), electron-electron (ee), and nuclei-electron (Ne). Thus, eFF is a mixed QM-classical mechanics method rather than a conventional force field method (in which electron motions are averaged out into ground state nuclear motions, i.e a single electronic state, and particle interactions are described via empirically parameterized interatomic potential functions). This makes eFF uniquely suited to simulate materials over a wide range of temperatures and pressures where electronically excited and ionized states of matter can occur and coexist. Furthermore, the interactions between particles -nuclei and electrons- reduce to the sum of a set of effective pairwise potentials in the eFF formulation. The *eff/cut* style computes the pairwise Coulomb interactions between nuclei and electrons (E_NN,E_Ne,E_ee), and the quantum-derived Pauli (E_PR) and Kinetic energy interactions potentials between electrons (E_KE) for a total energy expression given as,

$$U\left(R,r,s\right)=E_{NN}\left(R\right)+E_{Ne}\left(R,r,s\right)+E_{ee}\left(r,s\right)+E_{KE}\left(r,s\right)+E_{PR}\left(\uparrow\downarrow,S\right)$$

The individual terms are defined as follows:

$$\begin{aligned}
E_{KE} =& \frac{\hbar^2}{m_e}\sum_i \frac{3}{2s_i^2} \\
E_{NN} =& \frac{1}{4\pi\varepsilon_0}\sum_{i<j}\frac{Z_iZ_j}{R_{ij}} \\
E_{Ne} =& -\frac{1}{4\pi\varepsilon_0}\sum_{i,j}\frac{Z_i}{R_{ij}}Erf\left(\frac{\sqrt{2}R_{ij}}{s_j}\right) \\
E_{ee} =& \frac{1}{4\pi\varepsilon_0}\sum_{i<j}\frac{1}{r_{ij}}Erf\left(\frac{\sqrt{2}r_{ij}}{\sqrt{s_i^2+s_j^2}}\right) \\
E_{Pauli} =& \sum_{\sigma_i=\sigma_j}E\left(\uparrow\uparrow\right)_{ij}+\sum_{\sigma_i\neq\sigma_j}E\left(\uparrow\downarrow\right)_{ij}
\end{aligned}$$

where, s_i correspond to the electron sizes, the sigmas i's to the fixed spins of the electrons, Z_i to the charges on the

nuclei, R_ij to the distances between the nuclei or the nuclei and electrons, and r_ij to the distances between electrons. For additional details see *(Jaramillo-Botero)*.

The overall electrostatics energy is given in Hartree units of energy by default and can be modified by an energy-conversion constant, according to the units chosen (see *electron_units*). The cutoff Rc, given in Bohrs (by default), truncates the interaction distance. The recommended cutoff for this pair style should follow the minimum image criterion, i.e. half of the minimum unit cell length.

Style *eff/long* (not yet available) computes the same interactions as style *eff/cut* except that an additional damping factor is applied so it can be used in conjunction with the *kspace_style* command and its *ewald* or *pppm* option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

This potential is designed to be used with *atom_style electron* definitions, in order to handle the description of systems with interacting nuclei and explicit electrons.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- cutoff (distance units)

For *eff/cut*, the cutoff coefficient is optional. If it is not used (as in some of the examples above), the default global value specified in the pair_style command is used.

For *eff/long* (not yet available) no cutoff will be specified for an individual I,J type pair via the *pair_coeff* command. All type pairs use the same global cutoff specified in the pair_style command.

The *limit/eradius* and *pressure/evirials* keywords are optional. Neither or both must be specified. If not specified they are unset.

The *limit/eradius* keyword is used to restrain electron size from becoming excessively diffuse at very high temperatures were the Gaussian wave packet representation breaks down, and from expanding as free particles to infinite size. If unset, electron radius is free to increase without bounds. If set, a restraining harmonic potential of the form E = 1/2k_ss^2 for s > L_box/2, where k_s = 1 Hartrees/Bohr^2, is applied on the electron radius.

The *pressure/evirials* keyword is used to control between two types of pressure computation: if unset, the computed pressure does not include the electronic radial virials contributions to the total pressure (scalar or tensor). If set, the computed pressure will include the electronic radial virial contributions to the total pressure (scalar and tensor).

The *ecp* keyword is used to associate an ECP representation for a particular atom type. The ECP captures the orbital overlap between a core pseudo particle and valence electrons within the Pauli repulsion. A list of type:element-symbol pairs may be provided for all ECP representations, after the "ecp" keyword.

Note: Default ECP parameters are provided for C, N, O, Al, and Si. Users can modify these using the pair_coeff command as exemplified above. For this, the User must distinguish between two different functional forms supported, one that captures the orbital overlap assuming the s-type core interacts with an s-like valence electron (s-s) and another that assumes the interaction is s-p. For systems that exhibit significant p-character (e.g. C, N, O) the s-p form is recommended. The "s" ECP form requires 3 parameters and the "p" 5 parameters.

Note: there are two different pressures that can be reported for eFF when defining this pair_style, one (default) that considers electrons do not contribute radial virial components (i.e. electrons treated as incompressible 'rigid' spheres) and one that does. The radial electronic contributions to the virials are only tallied if the flexible pressure option is set, and this will affect both global and per-atom quantities. In principle, the true pressure of a system is somewhere in between the rigid and the flexible eFF pressures, but, for most cases, the difference between these two pressures

will not be significant over long-term averaged runs (i.e. even though the energy partitioning changes, the total energy remains similar).

Note: This implementation of eFF gives a reasonably accurate description for systems containing nuclei from Z = 1-6 in "all electron" representations. For systems with increasingly non-spherical electrons, Users should use the ECP representations. ECPs are now supported and validated for most of the 2nd and 3rd row elements of the p-block. Predefined parameters are provided for C, N, O, Al, and Si. The ECP captures the orbital overlap between the core and valence electrons (i.e. Pauli repulsion) with one of the functional forms:

$$
\begin{aligned}
E_{Pauli(ECP_s)} =& p_1 \exp\left(-\frac{p_2 r^2}{p_3 + s^2}\right) \\
E_{Pauli(ECP_p)} =& p_1 \left(\frac{2}{p_2/s + s/p_2}\right)(r - p_3 s)^2 \exp\left[-\frac{p_4 (r - p_3 s)^2}{p_5 + s^2}\right]
\end{aligned}
$$

Where the 1st form correspond to core interactions with s-type valence electrons and the 2nd to core interactions with p-type valence electrons.

The current version adds full support for models with fixed-core and ECP definitions. to enable larger timesteps (i.e. by avoiding the high frequency vibrational modes -translational and radial- of the 2 s electrons), and in the ECP case to reduce the increased orbital complexity in higher Z elements (up to Z<18). A fixed-core should be defined with a mass that includes the corresponding nuclear mass plus the 2 s electrons in atomic mass units (2x5.4857990943e-4), and a radius equivalent to that of minimized 1s electrons (see examples under /examples/USER/eff/fixed-core). An pseudo-core should be described with a mass that includes the corresponding nuclear mass, plus all the core electrons (i.e no outer shell electrons), and a radius equivalent to that of a corresponding minimized full-electron system. The charge for a pseudo-core atom should be given by the number of outer shell electrons.

In general, eFF excels at computing the properties of materials in extreme conditions and tracing the system dynamics over multi-picosecond timescales; this is particularly relevant where electron excitations can change significantly the nature of bonding in the system. It can capture with surprising accuracy the behavior of such systems because it describes consistently and in an unbiased manner many different kinds of bonds, including covalent, ionic, multicenter, ionic, and plasma, and how they interconvert and/or change when they become excited. eFF also excels in computing the relative thermochemistry of isodemic reactions and conformational changes, where the bonds of the reactants are of the same type as the bonds of the products. eFF assumes that kinetic energy differences dominate the overall exchange energy, which is true when the electrons present are nearly spherical and nodeless and valid for covalent compounds such as dense hydrogen, hydrocarbons, and diamond; alkali metals (e.g. lithium), alkali earth metals (e.g. beryllium) and semimetals such as boron; and various compounds containing ionic and/or multicenter bonds, such as boron dihydride.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the cutoff distance for the *eff/cut* style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

The *pair_modify* shift option is not relevant for these pair styles.

The *eff/long* (not yet available) style supports the *pair_modify* table option for tabulation of the short-range portion of the long-range Coulombic interaction.

These pair styles do not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

These pair styles write their information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

18.181.4 Restrictions

These pair styles will only be enabled if LAMMPS is built with the USER-EFF package. It will only be enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

These pair styles require that particles store electron attributes such as radius, radial velocity, and radial force, as defined by the *atom_style*. The *electron* atom style does all of this.

Thes pair styles require you to use the *comm_modify vel yes* command so that velocities are stored by ghost atoms.

18.181.5 Related commands

pair_coeff

18.181.6 Default

If not specified, limit_eradius = 0 and pressure_with_evirials = 0.

(Su) Su and Goddard, Excited Electron Dynamics Modeling of Warm Dense Matter, Phys Rev Lett, 99:185003 (2007).

(Jaramillo-Botero) Jaramillo-Botero, Su, Qi, Goddard, Large-scale, Long-term Non-adiabatic Electron Molecular Dynamics for Describing Material Properties and Phenomena in Extreme Environments, J Comp Chem, 32, 497-512 (2011).

18.182 pair_style eim command

18.183 pair_style eim/omp command

18.183.1 Syntax

```
pair_style style
```

- style = *eim*

18.183.2 Examples

```
pair_style eim
pair_coeff * * Na Cl ../potentials/ffield.eim Na Cl
pair_coeff * * Na Cl ffield.eim  Na Na Na Cl
pair_coeff * * Na Cl ../potentials/ffield.eim Cl NULL Na
```

18.183.3 Description

Style *eim* computes pairwise interactions for ionic compounds using embedded-ion method (EIM) potentials *(Zhou)*. The energy of the system E is given by

$$E = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=i_1}^{i_N}\phi_{ij}\left(r_{ij}\right) + \sum_{i=1}^{N}E_i\left(q_i,\sigma_i\right)$$

The first term is a double pairwise sum over the J neighbors of all I atoms, where ϕ_{ij} is a pair potential. The second term sums over the embedding energy E_i of atom I, which is a function of its charge q_i and the electrical potential σ_i at its location. E_i, q_i, and $sigma_i$ are calculated as

$$\begin{aligned} q_i =& \sum_{j=i_1}^{i_N}\eta_{ji}\left(r_{ij}\right) \\ \sigma_i =& \sum_{j=i_1}^{i_N}q_j\cdot\psi_{ij}\left(r_{ij}\right) \\ E_i\left(q_i,\sigma_i\right) =& \frac{1}{2}\cdot q_i\cdot\sigma_i \end{aligned}$$

where $\eta_{ji} isapairwisefunctiondescribingelectronflowfromatomItoatomJ, and : math$:psi_{ij}` is another pairwise function. The multi-body nature of the EIM potential is a result of the embedding energy term. A complete list of all the pair functions used in EIM is summarized below

$$\begin{aligned} \phi_{ij}\left(r\right) =& \begin{cases} \left[\frac{E_{b,ij}\beta_{ij}}{\beta_{ij}-\alpha_{ij}}\exp\left(-\alpha_{ij}\frac{r-r_{e,ij}}{r_{e,ij}}\right) - \frac{E_{b,ij}\alpha_{ij}}{\beta_{ij}-\alpha_{ij}}\exp\left(-\beta_{ij}\frac{r-r_{e,ij}}{r_{e,ij}}\right)\right]f_c\left(r,r_{e,ij},r_{c,\phi,ij}\right), & p_{ij}=1 \\ \left[\frac{E_{b,ij}\beta_{ij}}{\beta_{ij}-\alpha_{ij}}\left(\frac{r_{e,ij}}{r}\right)^{\alpha_{ij}} - \frac{E_{b,ij}\alpha_{ij}}{\beta_{ij}-\alpha_{ij}}\left(\frac{r_{e,ij}}{r}\right)^{\beta_{ij}}\right]f_c\left(r,r_{e,ij},r_{c,\phi,ij}\right), & p_{ij}=2 \end{cases} \\ \eta_{ji} =& A_{\eta,ij}\left(\chi_j-\chi_i\right)f_c\left(r,r_{s,\eta,ij},r_{c,\eta,ij}\right) \\ \psi_{ij}\left(r\right) =& A_{\psi,ij}\exp\left(-\zeta_{ij}r\right)f_c\left(r,r_{s,\psi,ij},r_{c,\psi,ij}\right) \\ f_c\left(r,r_p,r_c\right) =& 0.510204\mathrm{erfc}\left[\frac{1.64498\left(2r-r_p-r_c\right)}{r_c-r_p}\right] - 0.010204 \end{aligned}$$

Here $E_b, r_e, r_(c,\phi), \alpha, \beta, A_(\psi), \zeta, r_(s,\psi), r_(c,\psi), A_(\eta), r_(s,\eta), r_(c,\eta), \chi,$ and pair function type *p* are parameters, with subscripts *ij* indicating the two species of atoms in the atomic pair.

Note: Even though the EIM potential is treating atoms as charged ions, you should not use a LAMMPS *atom_style* that stores a charge on each atom and thus requires you to assign a charge to each atom, e.g. the *charge* or *full* atom styles. This is because the EIM potential infers the charge on an atom from the equation above for q_i; you do not assign charges explicitly.

All the EIM parameters are listed in a potential file which is specified by the *pair_coeff* command. This is an ASCII text file in a format described below. The "ffield.eim" file included in the "potentials" directory of the LAMMPS

distribution currently includes nine elements Li, Na, K, Rb, Cs, F, Cl, Br, and I. A system with any combination of these elements can be modeled. This file is parameterized in terms of LAMMPS *metal units*.

Note that unlike other potentials, cutoffs for EIM potentials are not set in the pair_style or pair_coeff command; they are specified in the EIM potential file itself. Likewise, the EIM potential file lists atomic masses; thus you do not need to use the *mass* command to specify them.

Only a single pair_coeff command is used with the *eim* style which specifies an EIM potential file and the element(s) to extract information for. The EIM elements are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- Elem1, Elem2, ...
- EIM potential file
- N element names = mapping of EIM elements to atom types

See the *pair_coeff* doc page for alternate ways to specify the path for the potential file.

As an example like one of those above, suppose you want to model a system with Na and Cl atoms. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Na, and the 4th to be Cl, you would use the following pair_coeff command:

```
pair_coeff * * Na Cl ffield.eim Na Na Na Cl
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The filename is the EIM potential file. The Na and Cl arguments (before the file name) are the two elements for which info will be extracted from the potential file. The first three trailing Na arguments map LAMMPS atom types 1,2,3 to the EIM Na element. The final Cl argument maps LAMMPS atom type 4 to the EIM Cl element.

If a mapping value is specified as NULL, the mapping is not performed. This can be used when an *eim* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

The ffield.eim file in the *potentials* directory of the LAMMPS distribution is formatted as follows:

Lines starting with # are comments and are ignored by LAMMPS. Lines starting with "global:" include three global values. The first value divides the cations from anions, i.e., any elements with electronegativity above this value are viewed as anions, and any elements with electronegativity below this value are viewed as cations. The second and third values are related to the cutoff function - i.e. the 0.510204, 1.64498, and 0.010204 shown in the above equation can be derived from these values.

Lines starting with "element:" are formatted as follows: name of element, atomic number, atomic mass, electronic negativity, atomic radius (LAMMPS ignores it), ionic radius (LAMMPS ignores it), cohesive energy (LAMMPS ignores it), and q0 (must be 0).

Lines starting with "pair:" are entered as: element 1, element 2, r_(c,phi), r_(c,phi) (redundant for historical reasons), E_b, r_e, alpha, beta, r_(c,eta), A_(eta), r_(s,eta), r_(c,psi), A_(psi), zeta, r_(s,psi), and p.

The lines in the file can be in any order; LAMMPS extracts the info it needs.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

18.183.4 Restrictions

This style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package.

18.183.5 Related commands

pair_coeff

Default: none

(Zhou) Zhou, submitted for publication (2010). Please contact Xiaowang Zhou (Sandia) for details via email at xzhou at sandia.gov.

18.184 pair_style exp6/rx command

18.185 pair_style exp6/rx/kk command

18.185.1 Syntax

```
pair_style exp6/rx cutoff ...
```

- cutoff = global cutoff for DPD interactions (distance units)
- weighting = fractional or molecular (optional)

18.185.2 Examples

```
pair_style exp6/rx 10.0
pair_style exp6/rx 10.0 fractional
pair_style exp6/rx 10.0 molecular
pair_coeff * * exp6.params h2o h2o exponent 1.0 1.0 10.0
pair_coeff * * exp6.params h2o 1fluid exponent 1.0 1.0 10.0
pair_coeff * * exp6.params 1fluid 1fluid exponent 1.0 1.0 10.0
pair_coeff * * exp6.params 1fluid 1fluid none 10.0
pair_coeff * * exp6.params 1fluid 1fluid polynomial filename 10.0
```

18.185.3 Description

Style *exp6/rx* is used in reaction DPD simulations, where the coarse-grained (CG) particles are composed of *m* species whose reaction rate kinetics are determined from a set of *n* reaction rate equations through the *fix rx* command. The species of one CG particle can interact with a species in a neighboring CG particle through a site-site interaction potential model. The *exp6/rx* style computes an exponential-6 potential given by

$$U_{ij}(r) = \frac{\epsilon}{\alpha - 6}\{6\exp[\alpha(1 - \frac{r_{ij}}{R_m})] - \alpha(\frac{R_m}{r_{ij}})^6\}$$

where the ϵ parameter determines the depth of the potential minimum located at R_m, and α determines the softness of the repulsion.

The coefficients must be defined for each species in a given particle type via the *pair_coeff* command as in the examples above, where the first argument is the filename that includes the exponential-6 parameters for each species. The file includes the species tag followed by the α, ϵ and R_m parameters. The format of the file is described below.

The second and third arguments specify the site-site interaction potential between two species contained within two different particles. The species tags must either correspond to the species defined in the reaction kinetics files specified with the *fix rx* command or they must correspond to the tag "1fluid", signifying interaction with a product species mixture determined through a one-fluid approximation. The interaction potential is weighted by the geometric average of either the mole fraction concentrations or the number of molecules associated with the interacting coarse-grained particles (see the *fractional* or *molecular* weighting pair style options). The coarse-grained potential is stored before and after the reaction kinetics solver is applied, where the difference is defined to be the internal chemical energy (uChem).

The fourth argument specifies the type of scaling that will be used to scale the EXP-6 parameters as reactions occur. Currently, there are three scaling options: *exponent*, *polynomial* and *none*.

Exponent scaling requires two additional arguments for scaling the R_m and ϵ parameters, respectively. The scaling factor is computed by phi^exponent, where phi is the number of molecules represented by the coarse-grain particle and exponent is specified as a pair coefficient argument for R_m and ϵ, respectively. The R_m and ϵ parameters are multiplied by the scaling factor to give the scaled interaction parameters for the CG particle.

Polynomial scaling requires a filename to be specified as a pair coeff argument. The file contains the coefficients to a fifth order polynomial for the α, ϵ and R_m parameters that depend upon phi (the number of molecules represented by the CG particle). The format of a polynomial file is provided below.

The *none* option to the scaling does not have any additional pair coeff arguments. This is equivalent to specifying the *exponent* option with R_m and ϵ exponents of 0.0 and 0.0, respectively.

The final argument specifies the interaction cutoff (optional).

The format of a tabulated file is as follows (without the parenthesized comments):

```
# exponential-6 parameters for various species      (one or more comment or blank␣
↪lines)

h2o  exp6  11.00 0.02 3.50                          (species, exp6, alpha, Rm,␣
↪epsilon)
no2  exp6  13.60 0.01 3.70
...
co2  exp6  13.00 0.03 3.20
```

The format of the polynomial scaling file as follows (without the parenthesized comments):

```
# POLYNOMIAL FILE          (one or more comment or blank lines)
```

```
#  General Functional Form:
#  A*phi^5 + B*phi^4 + C*phi^3 + D*phi^2 + E*phi + F
#
#  Parameter  A        B         C        D         E        F
                            (blank)
alpha        0.0000   0.00000   0.00008  0.04955  -0.73804  13.63201
epsilon      0.0000   0.00478  -0.06283  0.24486  -0.33737   2.60097
rm           0.0001  -0.00118  -0.00253  0.05812  -0.00509   1.50106
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections.

Following a blank line, the next N lines list the species and their corresponding parameters. The first argument is the species tag, the second argument is the exp6 tag, the 3rd argument is the α parameter (energy units), the 4th argument is the ϵ parameter (energy-distance^6 units), and the 5th argument is the R_m parameter (distance units). If a species tag of "1fluid" is listed as a pair coefficient, a one-fluid approximation is specified where a concentration-dependent combination of the parameters is computed through the following equations:

$$R_m^3 = \sum_a \sum_b x_a x_b R_{m,ab}^3$$
$$\epsilon = \frac{1}{R_m^3} \sum_a \sum_b x_a x_b \epsilon_{ab} R_{m,ab}^3$$
$$\alpha = \frac{1}{\epsilon R_m^3} \sum_a \sum_b x_a x_b \alpha_{ab} \epsilon_{ab} R_{m,ab}^3$$

where

$$\epsilon_{ab} = \sqrt{\epsilon_a \epsilon_b}$$
$$R_{m,ab} = \frac{R_{m,a} + R_{m,b}}{2}$$
$$\alpha_{ab} = \sqrt{\alpha_a \alpha_b}$$

and x_a and x_b are the mole fractions of a and b, respectively, which comprise the gas mixture.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the *pair_modify* shift option for the energy of the exp() and 1/r^6 portion of the pair interaction.

This style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure for the A,C terms in the pair interaction.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

18.185.4 Restrictions

This command is part of the USER-DPD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.185.5 Related commands

pair_coeff

Default: fractional weighting

18.186 pair_style extep command

18.186.1 Syntax

```
pair_style extep
```

18.186.2 Examples

```
pair_style extep
pair_coeff * * BN.extep B N
```

18.186.3 Description

Style *extep* computes the Extended Tersoff Potential (ExTeP) interactions as described in *(Los2017)*.

18.186.4 Restrictions

none

18.186.5 Related commands

"pair_tersoff" pair_tersoff.html

Default: none

(Los2017) J. H. Los et al. "Extended Tersoff potential for boron nitride: Energetics and elastic properties of pristine and defective h-BN", Phys. Rev. B 96 (184108), 2017.

18.187 pair_style lj/cut/soft command

18.188 pair_style lj/cut/soft/omp command

18.189 pair_style lj/cut/coul/cut/soft command

18.190 pair_style lj/cut/coul/cut/soft/omp command

18.191 pair_style lj/cut/coul/long/soft command

18.192 pair_style lj/cut/coul/long/soft/omp command

18.193 pair_style lj/cut/tip4p/long/soft command

18.194 pair_style lj/cut/tip4p/long/soft/omp command

18.195 pair_style lj/charmm/coul/long/soft command

18.196 pair_style lj/charmm/coul/long/soft/omp command

18.197 pair_style lj/class2/soft command

18.198 pair_style lj/class2/coul/cut/soft command

18.199 pair_style lj/class2/coul/long/soft command

18.200 pair_style coul/cut/soft command

18.201 pair_style coul/cut/soft/omp command

18.202 pair_style coul/long/soft command

18.203 pair_style coul/long/soft/omp command

18.204 pair_style tip4p/long/soft command

18.205 pair_style tip4p/long/soft/omp command

18.206 pair_style morse/soft command

18.206.1 Syntax

```
pair_style style args
```

- style = *lj/cut/soft* or *lj/cut/coul/cut/soft* or *lj/cut/coul/long/soft* or *lj/cut/tip4p/long/soft* or *lj/charmm/coul/long/soft* or *lj/class2/soft* or *lj/class2/coul/cut/soft* or *lj/class2/coul/long/soft* or *coul/cut/soft* or *coul/long/soft* or *tip4p/long/soft* or *morse/soft*
- args = list of arguments for a particular style

```
lj/cut/soft args = n alpha_lj cutoff
  n, alpha_LJ = parameters of soft-core potential
  cutoff = global cutoff for Lennard-Jones interactions (distance units)
lj/cut/coul/cut/soft args = n alpha_LJ alpha_C cutoff (cutoff2)
  n, alpha_LJ, alpha_C = parameters of soft-core potential
  cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
lj/cut/coul/long/soft args = n alpha_LJ alpha_C cutoff
  n, alpha_LJ, alpha_C = parameters of the soft-core potential
  cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
lj/cut/tip4p/long/soft args = otype htype btype atype qdist n alpha_LJ alpha_
↪C cutoff (cutoff2)
  otype,htype = atom types for TIP4P O and H
  btype,atype = bond and angle types for TIP4P waters
  qdist = distance from O atom to massless charge (distance units)
  n, alpha_LJ, alpha_C = parameters of the soft-core potential
  cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
lj/charmm/coul/long/soft args = n alpha_LJ alpha_C inner outer (cutoff)
  n, alpha_LJ, alpha_C = parameters of the soft-core potential
  inner, outer = global switching cutoffs for LJ (and Coulombic if only 5␣
↪args)
  cutoff = global cutoff for Coulombic (optional, outer is Coulombic cutoff␣
↪if only 5 args)
lj/class2/soft args = n alpha_lj cutoff
  n, alpha_LJ = parameters of soft-core potential
  cutoff = global cutoff for Lennard-Jones interactions (distance units)
lj/class2/coul/cut/soft args = n alpha_LJ alpha_C cutoff (cutoff2)
  n, alpha_LJ, alpha_C = parameters of soft-core potential
  cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
lj/class2/coul/long/soft args = n alpha_LJ alpha_C cutoff (cutoff2)
  n, alpha_LJ, alpha_C = parameters of soft-core potential
  cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
coul/cut/soft args = n alpha_C cutoff
  n, alpha_C = parameters of the soft-core potential
  cutoff = global cutoff for Coulomb interactions (distance units)
coul/long/soft args = n alpha_C cutoff
  n, alpha_C = parameters of the soft-core potential
  cutoff = global cutoff for Coulomb interactions (distance units)
tip4p/long/soft args = otype htype btype atype qdist n alpha_C cutoff
  otype,htype = atom types for TIP4P O and H
  btype,atype = bond and angle types for TIP4P waters
  qdist = distance from O atom to massless charge (distance units)
```

```
  n, alpha_C = parameters of the soft-core potential
  cutoff = global cutoff for Coulomb interactions (distance units)
morse/soft args = n lf cutoff
  n = soft-core parameter
  lf = transformation range is lf < lambda < 1
  cutoff = global cutoff for Morse interactions (distance units)
```

18.206.2 Examples

```
pair_style lj/cut/soft 2.0 0.5 9.5
pair_coeff * * 0.28 3.1 1.0
pair_coeff 1 1 0.28 3.1 1.0 9.5

pair_style lj/cut/coul/cut/soft 2.0 0.5 10.0 9.5
pair_style lj/cut/coul/cut/soft 2.0 0.5 10.0 9.5 9.5
pair_coeff * * 0.28 3.1 1.0
pair_coeff 1 1 0.28 3.1 0.5 10.0
pair_coeff 1 1 0.28 3.1 0.5 10.0 9.5

pair_style lj/cut/coul/long/soft 2.0 0.5 10.0 9.5
pair_style lj/cut/coul/long/soft 2.0 0.5 10.0 9.5 9.5
pair_coeff * * 0.28 3.1 1.0
pair_coeff 1 1 0.28 3.1 0.0 10.0
pair_coeff 1 1 0.28 3.1 0.0 10.0 9.5

pair_style lj/cut/tip4p/long/soft 1 2 7 8 0.15 2.0 0.5 10.0 9.8
pair_style lj/cut/tip4p/long/soft 1 2 7 8 0.15 2.0 0.5 10.0 9.8 9.5
pair_coeff * * 0.155 3.1536 1.0
pair_coeff 1 1 0.155 3.1536 1.0 9.5

pair_style lj/charmm/coul/long 2.0 0.5 10.0 8.0 10.0
pair_style lj/charmm/coul/long 2.0 0.5 10.0 8.0 10.0 9.0
pair_coeff * * 0.28 3.1 1.0
pair_coeff 1 1 0.28 3.1 1.0 0.14 3.1

pair_style lj/class2/coul/long/soft 2.0 0.5 10.0 9.5
pair_style lj/class2/coul/long/soft 2.0 0.5 10.0 9.5 9.5
pair_coeff * * 0.28 3.1 1.0
pair_coeff 1 1 0.28 3.1 0.0 10.0
pair_coeff 1 1 0.28 3.1 0.0 10.0 9.5

pair_style coul/long/soft 1.0 10.0 9.5
pair_coeff * * 1.0
pair_coeff 1 1 1.0 9.5

pair_style tip4p/long/soft 1 2 7 8 0.15 2.0 0.5 10.0 9.8
pair_coeff * * 1.0
pair_coeff 1 1 1.0 9.5

pair_style morse/soft 4 0.9 10.0
pair_coeff * * 100.0 2.0 1.5 1.0
pair_coeff 1 1 100.0 2.0 1.5 1.0 3.0
```

18.206.3 Description

These pair styles have a soft repulsive core, tunable by a parameter lambda, in order to avoid singularities during free energy calculations when sites are created or annihilated *(Beutler)*. When lambda tends to 0 the pair interaction vanishes with a soft repulsive core. When lambda tends to 1, the pair interaction approaches the normal, non-soft potential. These pair styles are suited for "alchemical" free energy calculations using the *fix adapt/fep* and *compute fep* commands.

The *lj/cut/soft* style and related sub-styles compute the 12-6 Lennard-Jones and Coulomb potentials modified by a soft core, with the functional form

$$E = \lambda^n 4\epsilon \left\{ \frac{1}{\left[\alpha_{\mathrm{LJ}}(1-\lambda)^2 + \left(\frac{r}{\sigma}\right)^6\right]^2} - \frac{1}{\alpha_{\mathrm{LJ}}(1-\lambda)^2 + \left(\frac{r}{\sigma}\right)^6} \right\} \qquad r < r_c$$

The *lj/class2/soft* style is a 9-6 potential with the exponent of the denominator of the first term in brackets taking the value 1.5 instead of 2 (other details differ, see the form of the potential in *pair_style lj/class2*).

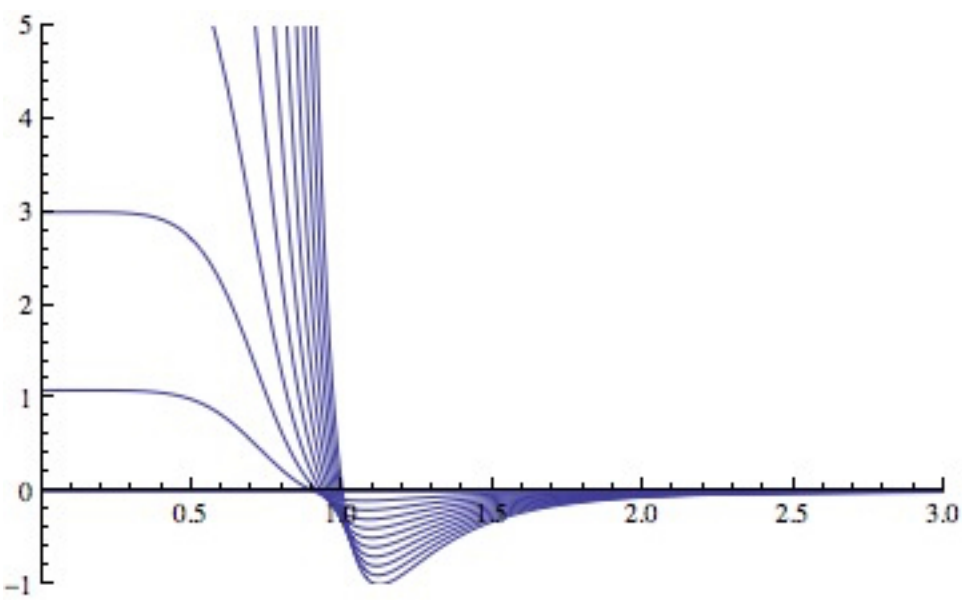
Coulomb interactions can also be damped with a soft core at short distance,

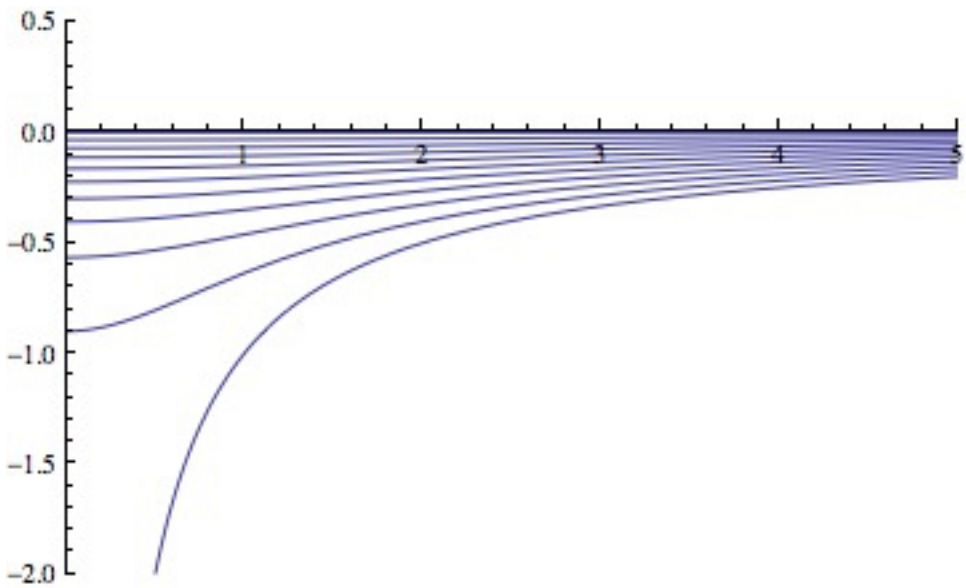
$$E = \lambda^n \frac{C q_i q_j}{\epsilon \left[\alpha_{\mathrm{C}}(1-\lambda)^2 + r^2\right]^{1/2}} \qquad r < r_c$$

In the Coulomb part C is an energy-conversion constant, q_i and q_j are the charges on the 2 atoms, and epsilon is the dielectric constant which can be set by the *dielectric* command.

The coefficient lambda is an activation parameter. When $\lambda = 1$ the pair potential is identical to a Lennard-Jones term or a Coulomb term or a combination of both. When $\lambda = 0$ the interactions are deactivated. The transition between these two extrema is smoothed by a soft repulsive core in order to avoid singularities in potential energy and forces when sites are created or annihilated and can overlap *(Beutler)*.

The parameters n, α_{LJ} and α_{C} are set in the *pair_style* command, before the cutoffs. Usual choices for the exponent are $n = 2$ or $n = 1$. For the remaining coefficients $\alpha_{\mathrm{LJ}} = 0.5$ and $\alpha_{\mathrm{C}} = 10$ A^2 are appropriate choices. Plots of the 12-6 LJ and Coulomb terms are shown below, for lambda ranging from 1 to 0 every 0.1.





For the *lj/cut/coul/cut/soft* or *lj/cut/coul/long/soft* pair styles, as well as for the equivalent *class2* versions, the following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- ϵ (energy units)
- σ (distance units)
- λ (activation parameter, between 0 and 1)
- cutoff1 (distance units)
- cutoff2 (distance units)

The latter two coefficients are optional. If not specified, the global LJ and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both LJ and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the LJ and Coulombic cutoffs for this type pair. You cannot specify 2 cutoffs for style *lj/cut/soft*, since it has no Coulombic terms. For the *coul/cut/soft* and *coul/long/soft* only lambda and the optional cutoff2 are to be specified.

Style *lj/cut/tip4p/long/soft* implements a soft-core version of the TIP4P water model. The usage of the TIP4P pair style is documented in the *pair_lj* styles. In the soft version the parameters n, α_{LJ} and α_{C} are set in the *pair_style* command, after the specific parameters of the TIP4P water model and before the cutoffs. The activation parameter lambda is supplied as an argument of the *pair_coeff* command, after epsilon and sigma and before the optional cutoffs.

Style *lj/charmm/coul/long/soft* implements a soft-core version of the modified 12-6 LJ potential used in CHARMM and documented in the *pair_style lj/charmm/coul/long* style. In the soft version the parameters n, α_{LJ} and α_{C} are set in the *pair_style* command, before the global cutoffs. The activation parameter lambda is introduced as an argument of the *pair_coeff* command, after ϵ and σ and before the optional eps14 and sigma14.

Style *lj/class2/soft* implements a soft-core version of the 9-6 potential in *pair_style lj/class2*. In the soft version the parameters n, α_{LJ} and α_{C} are set in the *pair_style* command, before the global cutoffs. The activation parameter lambda is introduced as an argument of the the *pair_coeff* command, after ϵ and σ and before the optional cutoffs.

The *coul/cut/soft*, *coul/long/soft* and *tip4p/long/soft* sub-styles are designed to be combined with other pair potentials via the *pair_style hybrid/overlay* command. This is because they have no repulsive core. Hence, if used by themselves, there will be no repulsion to keep two oppositely charged particles from overlapping each other. In this case, if $\lambda = 1$, a singularity may occur. These sub-styles are suitable to represent charges embedded in the Lennard-Jones radius of another site (for example hydrogen atoms in several water models).

Note: When using the soft-core Coulomb potentials with long-range solvers (*coul/long/soft*, *lj/cut/coul/long/soft*, etc.) in a free energy calculation in which sites holding electrostatic charges are being created or annihilated (using *fix adapt/fep* and *compute fep*) it is important to adapt both the λ activation parameter (from 0 to 1, or the reverse) and the value of the charge (from 0 to its final value, or the reverse). This ensures that long-range electrostatic terms (kspace) are correct. It is not necessary to use soft-core Coulomb potentials if the van der Waals site is present during the free-energy route, thus avoiding overlap of the charges. Examples are provided in the LAMMPS source directory tree, under examples/USER/fep.

Note: To avoid division by zero do not set $\sigma = 0$ in the *lj/cut/soft* and related styles; use the lambda parameter instead to activate/deactivate interactions, or use $\epsilon = 0$ and $\sigma = 1$. Alternatively, when sites do not interact though the Lennard-Jones term the *coul/long/soft* or similar sub-style can be used via the *pair_style hybrid/overlay* command.

The *morse/soft* variant modifies the *pair_morse* style at short range to have a soft core. The functional form differs from that of the *lj/soft* styles, and is instead given by:

$$
\begin{aligned}
s(\lambda) =& (1-\lambda)/(1-\lambda_f), \qquad B = -2De^{-2\alpha r_0}(e^{\alpha r_0}-1)/3 \\
E =& D_0\left[e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)}\right] + s(\lambda)Be^{-3\alpha(r-r_0)}, \qquad \lambda \geq \lambda_f, \quad r < r_c \\
E =& \left(D_0\left[e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)}\right] + Be^{-3\alpha(r-r_0)}\right)(\lambda/\lambda_f)^n, \qquad \lambda < \lambda_f, \quad r < r_c
\end{aligned}
$$

The *morse/soft* style requires the following pair coefficients:

- D_0 (energy units)
- α (1/distance units)
- r_0 (distance units)
- λ (unitless, between 0.0 and 1.0)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global morse cutoff is used.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, tail correction, restart info:

The different versions of the *lj/cut/soft* pair styles support mixing. For atom type pairs I,J and I != J, the ϵ and σ coefficients and cutoff distance for these pair style can be mixed. The default mix value is *geometric* for 12-6 styles.

The mixing rule for epsilon and sigma for *lj/class2/soft* 9-6 potentials is to use the *sixthpower* formulas. The *pair_modify mix* setting is thus ignored for class2 potentials for ϵ and σ. However it is still followed for mixing the cutoff distance. See the *pair_modify* command for details.

The *morse/soft* pair style does not support mixing. Thus, coefficients for all LJ pairs must be specified explicitly.

All of the pair styles with soft core support the *pair_modify* shift option for the energy of the Lennard-Jones portion of the pair interaction.

The different versions of the *lj/cut/soft* pair styles support the *pair_modify* tail option for adding a long-range tail correction to the energy and pressure for the Lennard-Jones portion of the pair interaction.

Note: The analytical form of the tail corrections for energy and pressure used in the *lj/cut/soft* potentials are approximate, being identical to that of the corresponding non-soft potentials scaled by a factor λ^n. The errors due to this approximation should be negligible. For example, for a cutoff of 2.5σ this approximation leads to maximum relative errors in tail corrections of the order of 1e-4 for energy and virial ($\alpha_{\mathrm{LJ}} = 0.5, n = 2$). The error vanishes when lambda approaches 0 or 1. Note that these are the errors affecting the long-range tail (itself a correction to the interaction energy) which includes other approximations, namely that the system is homogeneous (local density equal the average density) beyond the cutoff.

The *morse/soft* pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

All of these pair styles write information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

18.206.4 Restrictions

The pair styles with soft core are only enabled if LAMMPS was built with the USER-FEP package. The *long* versions also require the KSPACE package to be installed. The soft *tip4p* versions also require the MOLECULE package to be installed. These styles are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

18.206.5 Related commands

pair_coeff, *fix adapt*, *fix adapt/fep*, *compute fep*

Default: none

(Beutler) Beutler, Mark, van Schaik, Gerber, van Gunsteren, Chem Phys Lett, 222, 529 (1994).

18.207 pair_style gauss command

18.208 pair_style gauss/gpu command

18.209 pair_style gauss/omp command

18.210 pair_style gauss/cut command

18.211 pair_style gauss/cut/omp command

18.211.1 Syntax

```
pair_style gauss cutoff
pair_style gauss/cut cutoff
```

- cutoff = global cutoff for Gauss interactions (distance units)

18.211.2 Examples

```
pair_style gauss 12.0
pair_coeff * * 1.0 0.9
pair_coeff 1 4 1.0 0.9 10.0

pair_style gauss/cut 3.5
pair_coeff 1 4 0.2805 1.45 0.112
```

18.211.3 Description

Style *gauss* computes a tethering potential of the form

$$E = -A \exp(-Br^2) \qquad r < r_c$$

between an atom and its corresponding tether site which will typically be a frozen atom in the simulation. r_c is the cutoff.

The following coefficients must be defined for each pair of atom types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- A (energy units)
- B (1/distance^2 units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global cutoff is used.

Style *gauss/cut* computes a generalized Gaussian interaction potential between pairs of particles:

$$E = \frac{H}{\sigma_h \sqrt{2\pi}} \exp\left[-\frac{(r - r_{mh})^2}{2\sigma_h^2}\right]$$

where H determines together with the standard deviation σ_h the peak height of the Gaussian function, and r_{mh} the peak position. Examples of the use of the Gaussian potentials include implicit solvent simulations of salt ions *(Lenart)* and of surfactants *(Jusufi)*. In these instances the Gaussian potential mimics the hydration barrier between a pair of particles. The hydration barrier is located at r_{mh} and has a width of σ_h. The prefactor determines the height of the potential barrier.

The following coefficients must be defined for each pair of atom types via the *pair_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- H (energy * distance units)
- r_{mh} (distance units)
- σ_h (distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global cutoff is used.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the A, B, H, sigma_h, r_mh parameters, and the cutoff distance for these pair styles can be mixed: A (energy units) sqrt(1/B) (distance units, see below) H (energy units) sigma_h (distance units) r_mh (distance units) cutoff (distance units):ul

The default mix value is *geometric*. Only *arithmetic* and *geometric* mix values are supported. See the "pair_modify" command for details.

The A and H parameters are mixed using the same rules normally used to mix the "epsilon" parameter in a Lennard Jones interaction. The sigma_h, r_mh, and the cutoff distance are mixed using the same rules used to mix the "sigma" parameter in a Lennard Jones interaction. The B parameter is converted to a distance (sigma), before mixing (using sigma=B^-0.5), and converted back to a coefficient afterwards (using B=sigma^2). Negative A values are converted to positive A values (using abs(A)) before mixing, and converted back after mixing (by multiplying by min(sign(Ai),sign(Aj))). This way, if either particle is repulsive (if Ai<0 or Aj<0), then the default interaction between both particles will be repulsive.

The *gauss* style does not support the *pair_modify* shift option. There is no effect due to the Gaussian well beyond the cutoff; hence reasonable cutoffs need to be specified.

The *gauss/cut* style supports the *pair_modify* shift option for the energy of the Gauss-potential portion of the pair interaction.

The *pair_modify* table and tail options are not relevant for these pair styles.

These pair styles write their information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

The *gauss* pair style tallies an "occupancy" count of how many Gaussian-well sites have an atom within the distance at which the force is a maximum = sqrt(0.5/b). This quantity can be accessed via the *compute pair* command as a vector of values of length 1.

To print this quantity to the log file (with a descriptive column heading) the following commands could be included in an input script:

```
compute gauss all pair gauss
variable occ equal c_gauss[1]
thermo_style custom step temp epair v_occ
```

18.211.4 Restrictions

The *gauss/cut* style is part of the "user-misc" package. It is only enabled if LAMMPS is build with that package. See the *Build package* doc page for more info.

18.211.5 Related commands

pair_coeff, *pair_style coul/diel*

Default: none

(Lenart) Lenart , Jusufi, and Panagiotopoulos, J Chem Phys, 126, 044509 (2007).

(Jusufi) Jusufi, Hynninen, and Panagiotopoulos, J Phys Chem B, 112, 13783 (2008).

18.212 pair_style gayberne command

18.213 pair_style gayberne/gpu command

18.214 pair_style gayberne/intel command

18.215 pair_style gayberne/omp command

18.215.1 Syntax

```
pair_style gayberne gamma upsilon mu cutoff
```

- gamma = shift for potential minimum (typically 1)
- upsilon = exponent for eta orientation-dependent energy function
- mu = exponent for chi orientation-dependent energy function
- cutoff = global cutoff for interactions (distance units)

18.215.2 Examples

```
pair_style gayberne 1.0 1.0 1.0 10.0
pair_coeff * * 1.0 1.7 1.7 3.4 3.4 1.0 1.0 1.0
```

18.215.3 Description

The *gayberne* styles compute a Gay-Berne anisotropic LJ interaction *(Berardi)* between pairs of ellipsoidal particles or an ellipsoidal and spherical particle via the formulas

$$\begin{aligned} U(\mathbf{A}_1, \mathbf{A}_2, \mathbf{r}_{12}) =& U_r(\mathbf{A}_1, \mathbf{A}_2, \mathbf{r}_{12}, \gamma) \cdot \eta_{12}(\mathbf{A}_1, \mathbf{A}_2, \upsilon) \cdot \chi_{12}(\mathbf{A}_1, \mathbf{A}_2, \mathbf{r}_{12}, \mu) \\ U_r =& 4\epsilon(\varrho^{12} - \varrho^6) \\ \varrho =& \frac{\sigma}{h_{12} + \gamma\sigma} \end{aligned}$$

where A1 and A2 are the transformation matrices from the simulation box frame to the body frame and r_{12} is the center to center vector between the particles. U_r controls the shifted distance dependent interaction based on the distance of closest approach of the two particles (h_{12}) and the user-specified shift parameter gamma. When both particles are spherical, the formula reduces to the usual Lennard-Jones interaction (see details below for when Gay-Berne treats a particle as "spherical").

For large uniform molecules it has been shown that the energy parameters are approximately representable in terms of local contact curvatures *(Everaers)*:

$$\epsilon_a = \sigma \cdot \frac{a}{b \cdot c}; \epsilon_b = \sigma \cdot \frac{b}{a \cdot c}; \epsilon_c = \sigma \cdot \frac{c}{a \cdot b}$$

The variable names utilized as potential parameters are for the most part taken from *(Everaers)* in order to be consistent with the *RE-squared pair potential*. Details on the upsilon and mu parameters are given here.

More details of the Gay-Berne formulation are given in the references listed below and in this supplementary document.

Use of this pair style requires the NVE, NVT, or NPT fixes with the *asphere* extension (e.g. *fix nve/asphere*) in order to integrate particle rotation. Additionally, *atom_style ellipsoid* should be used since it defines the rotational state and the size and shape of each ellipsoidal particle.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- ϵ = well depth (energy units)
- σ = minimum effective particle radii (distance units)
- $\epsilon_{i,a}$ = relative well depth of type I for side-to-side interactions
- $\epsilon_{i,b}$ = relative well depth of type I for face-to-face interactions
- $\epsilon_{i,c}$ = relative well depth of type I for end-to-end interactions
- $\epsilon_{j,a}$ = relative well depth of type J for side-to-side interactions
- $\epsilon_{j,b}$ = relative well depth of type J for face-to-face interactions
- $\epsilon_{j,c}$ = relative well depth of type J for end-to-end interactions
- cutoff (distance units)

The last coefficient is optional. If not specified, the global cutoff specified in the pair_style command is used.

It is typical with the Gay-Berne potential to define σ as the minimum of the 3 shape diameters of the particles involved in an I,I interaction, though this is not required. Note that this is a different meaning for σ than the *pair_style resquared* potential uses.

The ϵ_i and ϵ_j coefficients are actually defined for atom types, not for pairs of atom types. Thus, in a series of pair_coeff commands, they only need to be specified once for each atom type.

Specifically, if any of $\epsilon_{i,a}$, $\epsilon_{i,b}$, $\epsilon_{i,c}$ are non-zero, the three values are assigned to atom type I. If all the ϵ_i values are zero, they are ignored. If any of $\epsilon_{j,a}$, $\epsilon_{j,b}$, $\epsilon_{j,c}$ are non-zero, the three values are assigned to atom type J. If all three epsilon_j values are zero, they are ignored. Thus the typical way to define the ϵ_i and ϵ_j coefficients is to list their values in "pair_coeff I J" commands when I = J, but set them to 0.0 when I != J. If you do list them when I != J, you should insure they are consistent with their values in other pair_coeff commands, since only the last setting will be in effect.

Note that if this potential is being used as a sub-style of *pair_style hybrid*, and there is no "pair_coeff I I" setting made for Gay-Berne for a particular type I (because I-I interactions are computed by another hybrid pair potential), then you still need to insure the ϵ a,b,c coefficients are assigned to that type. e.g. in a "pair_coeff I J" command.

Note: If the ϵ a = b = c for an atom type, and if the shape of the particle itself is spherical, meaning its 3 shape parameters are all the same, then the particle is treated as an LJ sphere by the Gay-Berne potential. This is significant because if two LJ spheres interact, then the simple Lennard-Jones formula is used to compute their interaction energy/force using the specified epsilon and sigma as the standard LJ parameters. This is much cheaper to compute than the full Gay-Berne formula. To treat the particle as a LJ sphere with sigma = D, you should normally set ϵ a = b = c = 1.0, set the pair_coeff $\sigma = D$, and also set the 3 shape parameters for the particle to D. The one exception is that if the 3 shape parameters are set to 0.0, which is a valid way in LAMMPS to specify a point particle, then the Gay-Berne potential will treat that as shape parameters of 1.0 (i.e. a LJ particle with $\sigma = 1$), since it requires finite-size particles. In this case you should still set the pair_coeff σ to 1.0 as well.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for this pair style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair styles supports the *pair_modify* shift option for the energy of the Lennard-Jones portion of the pair interaction, but only for sphere-sphere interactions. There is no shifting performed for ellipsoidal interactions due to the anisotropic dependence of the interaction.

The *pair_modify* table option is not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.215.4 Restrictions

The *gayberne* style is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

These pair style require that atoms store torque and a quaternion to represent their orientation, as defined by the *atom_style*. It also require they store a per-type *shape*. The particles cannot store a per-particle diameter.

This pair style requires that atoms be ellipsoids as defined by the *atom_style ellipsoid* command.

Particles acted on by the potential can be finite-size aspherical or spherical particles, or point particles. Spherical particles have all 3 of their shape parameters equal to each other. Point particles have all 3 of their shape parameters equal to 0.0.

The Gay-Berne potential does not become isotropic as r increases *(Everaers)*. The distance-of-closest-approach approximation used by LAMMPS becomes less accurate when high-aspect ratio ellipsoids are used.

18.215.5 Related commands

pair_coeff, *fix nve/asphere*, *compute temp/asphere*, *pair_style resquared*

Default: none

(Everaers) Everaers and Ejtehadi, Phys Rev E, 67, 041710 (2003).

(Berardi) Berardi, Fava, Zannoni, Chem Phys Lett, 297, 8-14 (1998). Berardi, Muccioli, Zannoni, J Chem Phys, 128, 024905 (2008).

(Perram) Perram and Rasmussen, Phys Rev E, 54, 6565-6572 (1996).

(Allen) Allen and Germano, Mol Phys 104, 3225-3235 (2006).

18.216 pair_style gran/hooke command

18.217 pair_style gran/hooke/omp command

18.218 pair_style gran/hooke/history command

18.219 pair_style gran/hooke/history/omp command

18.220 pair_style gran/hooke/history/kk command

18.221 pair_style gran/hertz/history command

18.222 pair_style gran/hertz/history/omp command

18.222.1 Syntax

```
pair_style style Kn Kt gamma_n gamma_t xmu dampflag
```

- style = *gran/hooke* or *gran/hooke/history* or *gran/hertz/history*
- Kn = elastic constant for normal particle repulsion (force/distance units or pressure units - see discussion below)
- Kt = elastic constant for tangential contact (force/distance units or pressure units - see discussion below)
- gamma_n = damping coefficient for collisions in normal direction (1/time units or 1/time-distance units - see discussion below)
- gamma_t = damping coefficient for collisions in tangential direction (1/time units or 1/time-distance units - see discussion below)
- xmu = static yield criterion (unitless value between 0.0 and 1.0e4)
- dampflag = 0 or 1 if tangential damping force is excluded or included

Note: Versions of LAMMPS before 9Jan09 had different style names for granular force fields. This is to emphasize the fact that the Hertzian equation has changed to model polydispersity more accurately. A side effect of the change is that the Kn, Kt, gamma_n, and gamma_t coefficients in the pair_style command must be specified with different values in order to reproduce calculations made with earlier versions of LAMMPS, even for monodisperse systems. See the NOTE below for details.

18.222.2 Examples

```
pair_style gran/hooke/history 200000.0 NULL 50.0 NULL 0.5 1
pair_style gran/hooke 200000.0 70000.0 50.0 30.0 0.5 0
```

18.222.3 Description

The *gran* styles use the following formulas for the frictional force between two granular particles, as described in *(Brilliantov)*, *(Silbert)*, and *(Zhang)*, when the distance r between two particles of radii Ri and Rj is less than their contact distance d = Ri + Rj. There is no force between the particles when r > d.

The two Hookean styles use this formula:

$$F_{hk} = (k_n \delta \mathbf{n}_{ij} - m_{eff} \gamma_n \mathbf{v}_n) - (k_t \mathbf{\Delta s}_t + m_{eff} \gamma_t \mathbf{v}_t)$$

The Hertzian style uses this formula:

$$F_{hz} = \sqrt{\delta} \sqrt{\frac{R_i R_j}{R_i + R_j}} F_{hk} = \sqrt{\delta} \sqrt{\frac{R_i R_j}{R_i + R_j}} \Big[(k_n \delta \mathbf{n}_{ij} - m_{eff}\ \gamma_n \mathbf{v}_n) - (k_t \mathbf{\Delta s}_t + m_{eff}\ \gamma_t \mathbf{v}_t) \Big]$$

In both equations the first parenthesized term is the normal force between the two particles and the second parenthesized term is the tangential force. The normal force has 2 terms, a contact force and a damping force. The tangential force also has 2 terms: a shear force and a damping force. The shear force is a "history" effect that accounts for the tangential displacement between the particles for the duration of the time they are in contact. This term is included in pair styles *hooke/history* and *hertz/history*, but is not included in pair style *hooke*. The tangential damping force term is included in all three pair styles if *dampflag* is set to 1; it is not included if *dampflag* is set to 0.

The other quantities in the equations are as follows:

- δ = d - r = overlap distance of 2 particles
- K_n = elastic constant for normal contact
- K_t = elastic constant for tangential contact
- γ_n = viscoelastic damping constant for normal contact
- γ_t = viscoelastic damping constant for tangential contact
- $m_{eff} = M_i M_j / (M_i + M_j) =$ effective mass of 2 particles of mass M_i and M_j
- $\mathbf{\Delta s}_t =$ tangential displacement vector between 2 particles which is truncated to satisfy a frictional yield criterion
- $n_{ij} =$ unit vector along the line connecting the centers of the 2 particles
- $V_n =$ normal component of the relative velocity of the 2 particles
- $V_t =$ tangential component of the relative velocity of the 2 particles

The K_n, K_t, γ_n, and γ_t coefficients are specified as parameters to the pair_style command. If a NULL is used for K_t, then a default value is used where $K_t = 2/7 K_n$. If a NULL is used for γ_t, then a default value is used where $\gamma_t = 1/2 \gamma_n$.

The interpretation and units for these 4 coefficients are different in the Hookean versus Hertzian equations.

The Hookean model is one where the normal push-back force for two overlapping particles is a linear function of the overlap distance. Thus the specified K_n is in units of (force/distance). Note that this push-back force is independent of absolute particle size (in the monodisperse case) and of the relative sizes of the two particles (in the polydisperse case). This model also applies to the other terms in the force equation so that the specified γ_n is in units of (1/time), K_t is in units of (force/distance), and γ_t is in units of (1/time).

The Hertzian model is one where the normal push-back force for two overlapping particles is proportional to the area of overlap of the two particles, and is thus a non-linear function of overlap distance. Thus Kn has units of force per area and is thus specified in units of (pressure). The effects of absolute particle size (monodispersity) and relative size (polydispersity) are captured in the radii-dependent pre-factors. When these pre-factors are carried through to the other terms in the force equation it means that the specified γ_n is in units of (1/(time*distance)), K_t is in units of (pressure), and γ_t is in units of (1/(time*distance)).

Note that in the Hookean case, K_n can be thought of as a linear spring constant with units of force/distance. In the Hertzian case, K_n is like a non-linear spring constant with units of force/area or pressure, and as shown in the *(Zhang)* paper, $K_n = 4G/(3(1-\nu))$ where ν = the Poisson ratio, G = shear modulus = $E/(2(1+\nu))$, and E = Young's modulus. Similarly, $K_t = 4G/(2-\nu)$. (NOTE: in an earlier version of the manual, we incorrectly stated that $K_t = 8G/(2-\nu)$.)

Thus in the Hertzian case K_n and K_t can be set to values that corresponds to properties of the material being modeled. This is also true in the Hookean case, except that a spring constant must be chosen that is appropriate for the absolute size of particles in the model. Since relative particle sizes are not accounted for, the Hookean styles may not be a suitable model for polydisperse systems.

Note: In versions of LAMMPS before 9Jan09, the equation for Hertzian interactions did not include the $\sqrt{r_i r_j/(r_i+r_j)}$ term and thus was not as accurate for polydisperse systems. For monodisperse systems, $\sqrt{r_i r_j/(r_i+r_j)}$ is a constant factor that effectively scales all 4 coefficients: $K_n, K_t, \gamma_n, \gamma_t$. Thus you can set the values of these 4 coefficients appropriately in the current code to reproduce the results of a previous Hertzian monodisperse calculation. For example, for the common case of a monodisperse system with particles of diameter 1, all 4 of these coefficients should now be set 2x larger than they were previously.

Xmu is also specified in the pair_style command and is the upper limit of the tangential force through the Coulomb criterion Ft = xmu*Fn, where Ft and Fn are the total tangential and normal force components in the formulas above. Thus in the Hookean case, the tangential force between 2 particles grows according to a tangential spring and dash-pot model until Ft/Fn = xmu and is then held at Ft = Fn*xmu until the particles lose contact. In the Hertzian case, a similar analogy holds, though the spring is no longer linear.

Note: Normally, xmu should be specified as a fractional value between 0.0 and 1.0, however LAMMPS allows large values (up to 1.0e4) to allow for modeling of systems which can sustain very large tangential forces.

The effective mass *m_eff* is given by the formula above for two isolated particles. If either particle is part of a rigid body, its mass is replaced by the mass of the rigid body in the formula above. This is determined by searching for a *fix rigid* command (or its variants).

For granular styles there are no additional coefficients to set for each pair of atom types via the *pair_coeff* command. All settings are global and are made via the pair_style command. However you must still use the *pair_coeff* for all pairs of granular atom types. For example the command

```
pair_coeff * *
```

should be used if all atoms in the simulation interact via a granular potential (i.e. one of the pair styles above is used). If a granular potential is used as a sub-style of *pair_style hybrid*, then specific atom types can be used in the pair_coeff command to determine which atoms interact via a granular potential.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

The *pair_modify* mix, shift, table, and tail options are not relevant for granular pair styles.

These pair styles write their information to *binary restart files*, so a pair_style command does not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

The single() function of these pair styles returns 0.0 for the energy of a pairwise interaction, since energy is not conserved in these dissipative potentials. It also returns only the normal component of the pairwise interaction force. However, the single() function also calculates 10 extra pairwise quantities. The first 3 are the components of the tangential force between particles I and J, acting on particle I. The 4th is the magnitude of this tangential force. The next 3 (5-7) are the components of the relative velocity in the normal direction (along the line joining the 2 sphere centers). The last 3 (8-10) the components of the relative velocity in the tangential direction.

These extra quantities can be accessed by the *compute pair/local* command, as *p1*, *p2*, . . . , *p10*.

18.222.4 Restrictions

All the granular pair styles are part of the GRANULAR package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

These pair styles require that atoms store torque and angular velocity (omega) as defined by the *atom_style*. They also require a per-particle radius is stored. The *sphere* atom style does all of this.

This pair style requires you to use the *comm_modify vel yes* command so that velocities are stored by ghost atoms.

These pair styles will not restart exactly when using the *read_restart* command, though they should provide statistically similar results. This is because the forces they compute depend on atom velocities. See the *read_restart* command for more details.

18.222.5 Related commands

pair_coeff

Default: none

(Brilliantov) Brilliantov, Spahn, Hertzsch, Poschel, Phys Rev E, 53, p 5382-5392 (1996).

(Silbert) Silbert, Ertas, Grest, Halsey, Levine, Plimpton, Phys Rev E, 64, p 051302 (2001).

(Zhang) Zhang and Makse, Phys Rev E, 72, p 011301 (2005).

18.223 pair_style granular command

18.223.1 Syntax

```
pair_style granular cutoff
```

- cutoff = global cutoff (optional). See discussion below.

18.223.2 Examples

```
pair_style granular
pair_coeff * * hooke 1000.0 50.0 tangential linear_nohistory 1.0 0.4 damping mass_
↪velocity

pair_style granular
pair_coeff * * hooke 1000.0 50.0 tangential linear_history 500.0 1.0 0.4 damping mass_
↪velocity

pair_style granular
pair_coeff * * hertz 1000.0 50.0 tangential mindlin 1000.0 1.0 0.4

pair_style granular
pair_coeff * * hertz/material 1e8 0.3 0.3 tangential mindlin_rescale NULL 1.0 0.4␣
↪damping tsuji

pair_style granular
pair_coeff 1 * jkr 1000.0 500.0 0.3 10 tangential mindlin 800.0 1.0 0.5 rolling sds␣
↪500.0 200.0 0.5 twisting marshall
pair_coeff 2 2 hertz 200.0 100.0 tangential linear_history 300.0 1.0 0.1 rolling sds␣
↪200.0 100.0 0.1 twisting marshall

pair_style granular
pair_coeff 1 1 dmt 1000.0 50.0 0.3 0.0 tangential mindlin NULL 0.5 0.5 rolling sds␣
↪500.0 200.0 0.5 twisting marshall
pair_coeff 2 2 dmt 1000.0 50.0 0.3 10.0 tangential mindlin NULL 0.5 0.1 rolling sds␣
↪500.0 200.0 0.1 twisting marshall
```

18.223.3 Description

The *granular* styles support a variety of options for the normal, tangential, rolling and twisting forces resulting from contact between two granular particles. This expands on the options offered by the *pair gran/** pair styles. The total computed forces and torques are the sum of various models selected for the normal, tangential, rolling and twisting modes of motion.

All model choices and parameters are entered in the *pair_coeff* command, as described below. Unlike e.g. *pair gran/hooke*, coefficient values are not global, but can be set to different values for different combinations of particle types, as determined by the *pair_coeff* command. If the contact model choice is the same for two particle types, the mixing for the cross-coefficients can be carried out automatically. This is shown in the last example, where model choices are the same for type 1 - type 1 as for type 2 - type2 interactions, but coefficients are different. In this case, the mixed coefficients for type 1 - type 2 interactions can be determined from mixing rules discussed below. For additional flexibility, coefficients as well as model forms can vary between particle types, as shown in the fourth example: type 1 - type 1 interactions are based on a Johnson-Kendall-Roberts normal contact model and 2-2 interactions are based on a DMT cohesive model (see below). In that example, 1-1 and 2-2 interactions have different model forms, in which

case mixing of coefficients cannot be determined, so 1-2 interactions must be explicitly defined via the *pair_coeff 1 ** command, otherwise an error would result.

The first required keyword for the *pair_coeff* command is the normal contact model. Currently supported options for normal contact models and their required arguments are:

1. *hooke* : k_n, η_{n0} (or e)
2. *hertz* : k_n, η_{n0} (or e)
3. *hertz/material* : E, η_{n0} (or e), ν
4. *dmt* : E, η_{n0} (or e), ν, γ
5. *jkr* : E, η_{n0} (or e), ν, γ

Here, k_n is spring stiffness (with units that depend on model choice, see below); η_{n0} is a damping prefactor (or, in its place a coefficient of restitution e, depending on the choice of damping mode, see below); E is Young's modulus in units of *force/length*^2, i.e. *pressure*; ν is Poisson's ratio and γ is a surface energy density, in units of *energy/length*^2.

For the *hooke* model, the normal, elastic component of force acting on particle *i* due to contact with particle *j* is given by:

$$\mathbf{F}_{ne,Hooke} = k_N \delta_{ij} \mathbf{n}$$

Where $\delta_{ij} = R_i + R_j - \|\mathbf{r}_{ij}\|$ is the particle overlap, R_i, R_j are the particle radii, $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ is the vector separating the two particle centers (note the i-j ordering so that F_{ne} is positive for repulsion), and $\mathbf{n} = \frac{\mathbf{r}_{ij}}{\|\mathbf{r}_{ij}\|}$. Therefore, for *hooke*, the units of the spring constant k_n are *force/distance*, or equivalently *mass/time*^2.

For the *hertz* model, the normal component of force is given by:

$$\mathbf{F}_{ne,Hertz} = k_N R_{eff}^{1/2} \delta_{ij}^{3/2} \mathbf{n}$$

Here, $R_{eff} = \frac{R_i R_j}{R_i + R_j}$ is the effective radius, denoted for simplicity as *R* from here on. For *hertz*, the units of the spring constant k_n are *force/length*^2, or equivalently *pressure*.

For the *hertz/material* model, the force is given by:

$$\mathbf{F}_{ne,Hertz/material} = \frac{4}{3} E_{eff} R_{eff}^{1/2} \delta_{ij}^{3/2} \mathbf{n}$$

Here, $E_{eff} = E = \left(\frac{1-\nu_i^2}{E_i} + \frac{1-\nu_j^2}{E_j} \right)^{-1}$ is the effective Young's modulus, with ν_i, ν_j the Poisson ratios of the particles of types *i* and *j*. Note that if the elastic modulus and the shear modulus of the two particles are the same, the *hertz/material* model is equivalent to the *hertz* model with $k_N = 4/3 E_{eff}$

The *dmt* model corresponds to the *(Derjaguin-Muller-Toporov)* cohesive model, where the force is simply Hertz with an additional attractive cohesion term:

$$\mathbf{F}_{ne,dmt} = \left(\frac{4}{3} E R^{1/2} \delta_{ij}^{3/2} - 4\pi\gamma R \right) \mathbf{n}$$

The *jkr* model is the *(Johnson-Kendall-Roberts)* model, where the force is computed as:

$$\mathbf{F}_{ne,jkr} = \left(\frac{4Ea^3}{3R} - 2\pi a^2 \sqrt{\frac{4\gamma E}{\pi a}} \right) \mathbf{n}$$

Here, *a* is the radius of the contact zone, related to the overlap δ according to:

$$\delta = a^2/R - 2\sqrt{\pi\gamma a/E}$$

LAMMPS internally inverts the equation above to solve for *a* in terms of δ, then solves for the force in the previous equation. Additionally, note that the JKR model allows for a tensile force beyond contact (i.e. for $\delta < 0$), up to a maximum of $3\pi\gamma R$ (also known as the 'pull-off' force). Note that this is a hysteretic effect, where particles that are not contacting initially will not experience force until they come into contact $\delta \geq 0$; as they move apart and ($\delta < 0$), they experience a tensile force up to $3\pi\gamma R$, at which point they lose contact.

In addition, the normal force is augmented by a damping term of the following general form:

$$\mathbf{F}_{n,damp} = -\eta_n \mathbf{v}_{n,rel}$$

Here, $\mathbf{v}_{n,rel} = (\mathbf{v}_j - \mathbf{v}_i) \cdot \mathbf{nn}$ is the component of relative velocity along $\mathbf{n}$.

The optional *damping* keyword to the *pair_coeff* command followed by a keyword determines the model form of the damping factor η_n, and the interpretation of the η_{n0} or e coefficients specified as part of the normal contact model settings. The *damping* keyword and corresponding model form selection may be appended anywhere in the *pair coeff* command. Note that the choice of damping model affects both the normal and tangential damping (and depending on other settings, potentially also the twisting damping). The options for the damping model currently supported are:

1. *velocity*
2. *mass_velocity*
3. *viscoelastic*
4. *tsuji*

If the *damping* keyword is not specified, the *viscoelastic* model is used by default.

For *damping velocity*, the normal damping is simply equal to the user-specified damping coefficient in the *normal* model:

$$\eta_n = \eta_{n0}$$

Here, η_{n0} is the damping coefficient specified for the normal contact model, in units of *mass/time*.

For *damping mass_velocity*, the normal damping is given by:

$$\eta_n = \eta_{n0} m_{eff}$$

Here, η_{n0} is the damping coefficient specified for the normal contact model, in units of *mass/time* and $m_{eff} = m_i m_j/(m_i + m_j)$ is the effective mass. Use *damping mass_velocity* to reproduce the damping behavior of *pair gran/hooke/**.

The *damping viscoelastic* model is based on the viscoelastic treatment of *(Brilliantov et al)*, where the normal damping is given by:

$$\eta_n = \eta_{n0}\, a m_{eff}$$

Here, *a* is the contact radius, given by $a = \sqrt{R\delta}$ for all models except *jkr*, for which it is given implicitly according to $\delta = a^2/R - 2\sqrt{\pi\gamma a/E}$. For *damping viscoelastic*, η_{n0} is in units of 1/(*time***distance*).

The *tsuji* model is based on the work of *(Tsuji et al)*. Here, the damping coefficient specified as part of the normal model is interpreted as a restitution coefficient e. The damping constant η_n is given by:

$$\eta_n = \alpha (m_{eff} k_n)^{1/2}$$

For normal contact models based on material parameters, $k_n = 4/3Ea$. The parameter α is related to the restitution coefficient *e* according to:

$$\alpha = 1.2728 - 4.2783e + 11.087e^2 - 22.348e^3 + 27.467e^4 - 18.022e^5 + 4.8218e^6$$

The dimensionless coefficient of restitution e specified as part of the normal contact model parameters should be between 0 and 1, but no error check is performed on this.

The total normal force is computed as the sum of the elastic and damping components:

$$\mathbf{F}_n = \mathbf{F}_{ne} + \mathbf{F}_{n,damp}$$

The *pair_coeff* command also requires specification of the tangential contact model. The required keyword *tangential* is expected, followed by the model choice and associated parameters. Currently supported tangential model choices and their expected parameters are as follows:

1. *linear_nohistory* : $x_{\gamma,t}$, μ_s
2. *linear_history* : k_t, $x_{\gamma,t}$, μ_s
3. *mindlin* : k_t or NULL, $x_{\gamma,t}$, μ_s
4. *mindlin_rescale* : k_t or NULL, $x_{\gamma,t}$, μ_s

Here, $x_{\gamma,t}$ is a dimensionless multiplier for the normal damping η_n that determines the magnitude of the tangential damping, μ_t is the tangential (or sliding) friction coefficient, and k_t is the tangential stiffness coefficient.

For *tangential linear_nohistory*, a simple velocity-dependent Coulomb friction criterion is used, which mimics the behavior of the *pair gran/hooke* style. The tangential force (mathbf{F}_t) is given by:

$$\mathbf{F}_t = -min(\mu_t F_{n0}, \|\mathbf{F}_{\mathrm{t,damp}}\|)\mathbf{t}$$

The tangential damping force $\mathbf{F}_{\mathrm{t,damp}}$ is given by:

$$\mathbf{F}_{\mathrm{t,damp}} = -\eta_t \mathbf{v}_{t,rel}$$

The tangential damping prefactor η_t is calculated by scaling the normal damping η_n (see above):

$$\eta_t = -x_{\gamma,t}\eta_n$$

The normal damping prefactor η_n is determined by the choice of the *damping* keyword, as discussed above. Thus, the *damping* keyword also affects the tangential damping. The parameter $x_{\gamma,t}$ is a scaling coefficient. Several works in the literature use $x_{\gamma,t} = 1$ (*Marshall*, *Tsuji et al*, *Silbert et al*). The relative tangential velocity at the point of contact is given by $\mathbf{v}_{t,rel} = \mathbf{v}_t - (R_i\Omega_i + R_j\Omega_j) \times \mathbf{n}$, where $\mathbf{v}_t = \mathbf{v}_r - \mathbf{v}_r \cdot \mathbf{n}n$, $\mathbf{v}_r = \mathbf{v}_j - \mathbf{v}_i$. The direction of the applied force is $\mathbf{t} = \mathbf{v_{t,rel}}/\|\mathbf{v_{t,rel}}\|$.

The normal force value F_{n0} used to compute the critical force depends on the form of the contact model. For non-cohesive models (*hertz*, *hertz/material*, *hooke*), it is given by the magnitude of the normal force:

$$F_{n0} = \|\mathbf{F}_n\|$$

For cohesive models such as *jkr* and *dmt*, the critical force is adjusted so that the critical tangential force approaches $\mu_t F_{pulloff}$, see *Marshall*, equation 43, and *Thornton*. For both models, F_{n0} takes the form:

$$F_{n0} = \|\mathbf{F}_n e + 2F_{pulloff}\|$$

Where $F_{pulloff} = 3\pi\gamma R$ for *jkr*, and $F_{pulloff} = 4\pi\gamma R$ for *dmt*.

The remaining tangential options all use accumulated tangential displacement (i.e. contact history). This is discussed below in the context of the *linear_history* option, but the same treatment of the accumulated displacement applies to the other options as well.

For *tangential linear_history*, the tangential force is given by:

$$\mathbf{F}_t = -min(\mu_t F_{n0}, \| - k_t \xi + \mathbf{F}_{\mathrm{t,damp}} \|)\mathbf{t}$$

Here, ξ is the tangential displacement accumulated during the entire duration of the contact:

$$\xi = \int_{t0}^{t} \mathbf{v}_{t,rel}(\tau) \mathrm{d}\tau$$

This accumulated tangential displacement must be adjusted to account for changes in the frame of reference of the contacting pair of particles during contact. This occurs due to the overall motion of the contacting particles in a rigid-body-like fashion during the duration of the contact. There are two modes of motion that are relevant: the 'tumbling' rotation of the contacting pair, which changes the orientation of the plane in which tangential displacement occurs; and 'spinning' rotation of the contacting pair about the vector connecting their centers of mass ($\mathbf{n}$). Corrections due to the former mode of motion are made by rotating the accumulated displacement into the plane that is tangential to the contact vector at each step, or equivalently removing any component of the tangential displacement that lies along $\mathbf{n}$, and rescaling to preserve the magnitude. This follows the discussion in *Luding*, see equation 17 and relevant discussion in that work:

$$\xi = (\xi' - (\mathbf{n} \cdot \xi')\mathbf{n}) \frac{\|\xi'\|}{\|\xi'\| - \mathbf{n} \cdot \xi'}$$

Here, ξ' is the accumulated displacement prior to the current time step and ξ is the corrected displacement. Corrections to the displacement due to the second mode of motion described above (rotations about $\mathbf{n}$) are not currently implemented, but are expected to be minor for most simulations.

Furthermore, when the tangential force exceeds the critical force, the tangential displacement is re-scaled to match the value for the critical force (see *Luding*, equation 20 and related discussion):

$$\xi = -\frac{1}{k_t} \left(\mu_t F_{n0} \mathbf{t} + \mathbf{F}_{t,damp} \right)$$

The tangential force is added to the total normal force (elastic plus damping) to produce the total force on the particle. The tangential force also acts at the contact point (defined as the center of the overlap region) to induce a torque on each particle according to:

$$\tau_i = -(R_i - 0.5\delta)\mathbf{n} \times \mathbf{F}_t$$

$$\tau_j = -(R_j - 0.5\delta)\mathbf{n} \times \mathbf{F}_t$$

For *tangential mindlin*, the *Mindlin* no-slip solution is used, which differs from the *linear_history* option by an additional factor of *a*, the radius of the contact region. The tangential force is given by:

$$\mathbf{F}_t = -min(\mu_t F_{n0}, \| - k_t a \xi + \mathbf{F}_{\mathrm{t,damp}} \|)\mathbf{t}$$

Here, a is the radius of the contact region, given by $a = \sqrt{R\delta}$ for all normal contact models, except for *jkr*, where it is given implicitly by $\delta = a^2/R - 2\sqrt{\pi\gamma a/E}$, see discussion above. To match the Mindlin solution, one should set $k_t = 4G/(2-\nu)$, where G is the shear modulus, related to Young's modulus E by $G = E/(2(1+\nu))$, where ν is Poisson's ratio. This can also be achieved by specifying *NULL* for k_t, in which case a normal contact model that specifies material parameters E and ν is required (e.g. *hertz/material*, *dmt* or *jkr*). In this case, mixing of the shear modulus for different particle types *i* and *j* is done according to:

$$1/G = 2(2-\nu_i)(1+\nu_i)/E_i + 2(2-\nu_j)(1+\nu_j)/E_j$$

The *mindlin_rescale* option uses the same form as *mindlin*, but the magnitude of the tangential displacement is re-scaled as the contact unloads, i.e. if $a < a_{t_{n-1}}$:

$$\xi = \xi_{\mathbf{t_{n-1}}} \frac{a}{a_{t_{n-1}}}$$

Here, t_{n-1} indicates the value at the previous time step. This rescaling accounts for the fact that a decrease in the contact area upon unloading leads to the contact being unable to support the previous tangential loading, and spurious energy is created without the rescaling above (*Walton*). See also discussion in *Thornton et al, 2013* , particularly equation 18(b) of that work and associated discussion.

The optional *rolling* keyword enables rolling friction, which resists pure rolling motion of particles. The options currently supported are:

1. *none*
2. *sds* : k_{roll}, γ_{roll}, μ_{roll}

If the *rolling* keyword is not specified, the model defaults to *none*.

For *rolling sds*, rolling friction is computed via a spring-dashpot-slider, using a 'pseudo-force' formulation, as detailed by *Luding*. Unlike the formulation in *Marshall*, this allows for the required adjustment of rolling displacement due to changes in the frame of reference of the contacting pair. The rolling pseudo-force is computed analogously to the tangential force:

$$\mathbf{F}_{roll,0} = k_{roll}\xi_{roll} - \gamma_{roll}\mathbf{v}_{roll}$$

Here, $\mathbf{v}_{roll} = -R(\mathbf{\Omega}_i - \mathbf{\Omega}_j) \times \mathbf{n}$ is the relative rolling velocity, as given in *Wang et al* and *Luding*. This differs from the expressions given by *Kuhn and Bagi* and used in *Marshall*; see *Wang et al* for details. The rolling displacement is given by:

$$\xi_{roll} = \int_{t_0}^{t} \mathbf{v}_{roll}(\tau)\mathrm{d}\tau$$

A Coulomb friction criterion truncates the rolling pseudo-force if it exceeds a critical value:

$$\mathbf{F}_{roll} = min(\mu_{roll}F_{n,0}, \|\mathbf{F}_{roll,0}\|)\mathbf{k}$$

Here, $\mathbf{k} = \mathbf{v}_{roll}/\|\mathbf{v}_{roll}\|$ is the direction of the pseudo-force. As with tangential displacement, the rolling displacement is rescaled when the critical force is exceeded, so that the spring length corresponds the critical force. Additionally, the displacement is adjusted to account for rotations of the frame of reference of the two contacting particles in a manner analogous to the tangential displacement.

The rolling pseudo-force does not contribute to the total force on either particle (hence 'pseudo'), but acts only to induce an equal and opposite torque on each particle, according to:

$$\tau_{roll,i} = R_{eff}\mathbf{n} \times \mathbf{F}_{roll}$$

$$\tau_{roll,j} = -\tau_{roll,i}$$

The optional *twisting* keyword enables twisting friction, which resists rotation of two contacting particles about the vector $\mathbf{n}$ that connects their centers. The options currently supported are:

1. *none*
2. *sds* : k_{twist}, γ_{twist}, μ_{twist}
3. *marshall*

If the *twisting* keyword is not specified, the model defaults to *none*.

For both *twisting sds* and *twisting marshall*, a history-dependent spring-dashpot-slider is used to compute the twisting torque. Because twisting displacement is a scalar, there is no need to adjust for changes in the frame of reference due to rotations of the particle pair. The formulation in *Marshall* therefore provides the most straightforward treatment:

$$\tau_{twist,0} = -k_{twist}\xi_{twist} - \gamma_{twist}\Omega_{twist}$$

Here $\xi_{twist} = \int_{t_0}^{t} \Omega_{twist}(\tau)\mathrm{d}\tau$ is the twisting angular displacement, and $\Omega_{twist} = (\mathbf{\Omega}_i - \mathbf{\Omega}_j)\cdot\mathbf{n}$ is the relative twisting angular velocity. The torque is then truncated according to:

$$\tau_{twist} = min(\mu_{twist}F_{n,0}, \tau_{twist,0})$$

Similar to the sliding and rolling displacement, the angular displacement is rescaled so that it corresponds to the critical value if the twisting torque exceeds this critical value:

$$\xi_{twist} = \frac{1}{k_{twist}}(\mu_{twist}F_{n,0}sgn(\Omega_{twist}) - \gamma_{twist}\Omega_{twist})$$

For *twisting sds*, the coefficients $k_{twist}, \gamma_{twist}$ and μ_{twist} are simply the user input parameters that follow the *twisting sds* keywords in the *pair_coeff* command.

For *twisting_marshall*, the coefficients are expressed in terms of sliding friction coefficients, as discussed in *Marshall* (see equations 32 and 33 of that work):

$$k_{twist} = 0.5k_t a^2$$

$$\eta_{twist} = 0.5\eta_t a^2$$

$$\mu_{twist} = \frac{2}{3}a\mu_t$$

Finally, the twisting torque on each particle is given by:

$$\tau_{twist,i} = \tau_{twist}\mathbf{n}$$

$$\tau_{twist,j} = -\tau_{twist,i}$$

The *granular* pair style can reproduce the behavior of the *pair gran/** styles with the appropriate settings (some very minor differences can be expected due to corrections in displacement history frame-of-reference, and the application of the torque at the center of the contact rather than at each particle). The first example above is equivalent to *pair gran/hooke 1000.0 NULL 50.0 50.0 0.4 1*. The second example is equivalent to *pair gran/hooke/history 1000.0 500.0 50.0 50.0 0.4 1*. The third example is equivalent to *pair gran/hertz/history 1000.0 500.0 50.0 50.0 0.4 1*.

LAMMPS automatically sets pairwise cutoff values for *pair_style granular* based on particle radii (and in the case of *jkr* pull-off distances). In the vast majority of situations, this is adequate. However, a cutoff value can optionally be appended to the *pair_style granular* command to specify a global cutoff (i.e. a cutoff for all atom types). Additionally, the optional *cutoff* keyword can be passed to the *pair_coeff* command, followed by a cutoff value. This will set a pairwise cutoff for the atom types in the *pair_coeff* command. These options may be useful in some rare cases where the automatic cutoff determination is not sufficient, e.g. if particle diameters are being modified via the *fix adapt* command. In that case, the global cutoff specified as part of the *pair_style granular* command is applied to all atom types, unless it is overridden for a given atom type combination by the *cutoff* value specified in the *pair coeff* command. If *cutoff* is only specified in the *pair coeff* command and no global cutoff is appended to the *pair_style granular* command, then LAMMPS will use that cutoff for the specified atom type combination, and automatically set pairwise cutoffs for the remaining atom types.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

The *pair_modify* mix, shift, table, and tail options are not relevant for granular pair styles.

Mixing of coefficients is carried out using geometric averaging for most quantities, e.g. if friction coefficient for type 1-type 1 interactions is set to μ_1, and friction coefficient for type 2-type 2 interactions is set to μ_2, the friction coefficient for type1-type2 interactions is computed as $\sqrt{\mu_1 \mu_2}$ (unless explicitly specified to a different value by a *pair_coeff 1 2 ...* command). The exception to this is elastic modulus, only applicable to *hertz/material*, *dmt* and *jkr* normal contact models. In that case, the effective elastic modulus is computed as:

$$E_{eff,ij} = \left(\frac{1-\nu_i^2}{E_i} + \frac{1-\nu_j^2}{E_j} \right)^{-1}$$

If the *i-j* coefficients E_{ij} and ν_{ij} are explicitly specified, the effective modulus is computed as:

$$E_{eff,ij} = \left(\frac{1-\nu_{ij}^2}{E_{ij}} + \frac{1-\nu_{ij}^2}{E_{ij}} \right)^{-1}$$

or

$$E_{eff,ij} = \frac{E_{ij}}{2(1-\nu_{ij})}$$

These pair styles write their information to *binary restart files*, so a pair_style command does not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

The single() function of these pair styles returns 0.0 for the energy of a pairwise interaction, since energy is not conserved in these dissipative potentials. It also returns only the normal component of the pairwise interaction force. However, the single() function also calculates 12 extra pairwise quantities. The first 3 are the components of the tangential force between particles I and J, acting on particle I. The 4th is the magnitude of this tangential force. The next 3 (5-7) are the components of the rolling torque acting on particle I. The next entry (8) is the magnitude of the rolling torque. The next entry (9) is the magnitude of the twisting torque acting about the vector connecting the two particle centers. The last 3 (10-12) are the components of the vector connecting the centers of the two particles (x_I - x_J).

These extra quantities can be accessed by the *compute pair/local* command, as *p1*, *p2*, ..., *p12*.

18.223.4 Restrictions

All the granular pair styles are part of the GRANULAR package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

These pair styles require that atoms store torque and angular velocity (omega) as defined by the *atom_style*. They also require a per-particle radius is stored. The *sphere* atom style does all of this.

This pair style requires you to use the *comm_modify vel yes* command so that velocities are stored by ghost atoms.

These pair styles will not restart exactly when using the *read_restart* command, though they should provide statistically similar results. This is because the forces they compute depend on atom velocities. See the *read_restart* command for more details.

18.223.5 Related commands

*pair_coeff pair gran/**

18.223.6 Default

For the *pair_coeff* settings: *damping viscoelastic*, *rolling none*, *twisting none*.

References:

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(Otis R. Walton) Walton, O.R., Personal Communication

18.224 pair_style lj/gromacs command

18.225 pair_style lj/gromacs/gpu command

18.226 pair_style lj/gromacs/kk command

18.227 pair_style lj/gromacs/omp command

18.228 pair_style lj/gromacs/coul/gromacs command

18.229 pair_style lj/gromacs/coul/gromacs/kk command

18.230 pair_style lj/gromacs/coul/gromacs/omp command

18.230.1 Syntax

```
pair_style style args
```

- style = *lj/gromacs* or *lj/gromacs/coul/gromacs*
- args = list of arguments for a particular style

```
lj/gromacs args = inner outer
  inner, outer = global switching cutoffs for Lennard Jones
lj/gromacs/coul/gromacs args = inner outer (inner2) (outer2)
  inner, outer = global switching cutoffs for Lennard Jones (and Coulombic if␣
↪only 2 args)
  inner2, outer2 = global switching cutoffs for Coulombic (optional)
```

18.230.2 Examples

```
pair_style lj/gromacs 9.0 12.0
pair_coeff * * 100.0 2.0
pair_coeff 2 2 100.0 2.0 8.0 10.0

pair_style lj/gromacs/coul/gromacs 9.0 12.0
pair_style lj/gromacs/coul/gromacs 8.0 10.0 7.0 9.0
pair_coeff * * 100.0 2.0
```

18.230.3 Description

The *lj/gromacs* styles compute shifted LJ and Coulombic interactions with an additional switching function S(r) that ramps the energy and force smoothly to zero between an inner and outer cutoff. It is a commonly used potential in the GROMACS MD code and for the coarse-grained models of *(Marrink)*.

$$
\begin{aligned}
E_{LJ} =& 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] + S_{LJ}(r) \qquad r < r_c \\
E_C =& \frac{C q_i q_j}{\epsilon r} + S_C(r) \qquad r < r_c \\
S(r) =& C \qquad r < r_1 \\
S(r) =& \frac{A}{3}(r-r_1)^3 + \frac{B}{4}(r-r_1)^4 + C \qquad r_1 < r < r_c \\
A =& (-3E'(r_c) + (r_c - r_1)E''(r_c))/(r_c - r_1)^2 \\
B =& (2E'(r_c) - (r_c - r_1)E''(r_c))/(r_c - r_1)^3 \\
C =& -E(r_c) + \frac{1}{2}(r_c - r_1)E'(r_c) - \frac{1}{12}(r_c - r_1)^2 E''(r_c)
\end{aligned}
$$

r_1 is the inner cutoff; r_c is the outer cutoff. The coefficients A, B, and C are computed by LAMMPS to perform the shifting and smoothing. The function S(r) is actually applied once to each term of the LJ formula and once to the Coulombic formula, so there are 2 or 3 sets of A,B,C coefficients depending on which pair_style is used. The boundary conditions applied to the smoothing function are as follows: $S'(r_1) = S''(r_1) = 0, S(r_c) = -E(r_c), S'(r_c) = -E'(r_c)$, and $S''(r_c) = -E''(r_c)$, where E(r) is the corresponding term in the LJ or Coulombic potential energy function. Single and double primes denote first and second derivatives with respect to r, respectively.

The inner and outer cutoff for the LJ and Coulombic terms can be the same or different depending on whether 2 or 4 arguments are used in the pair_style command. The inner LJ cutoff must be > 0, but the inner Coulombic cutoff can be >= 0.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- ϵ (energy units)
- σ (distance units)
- inner (distance units)
- outer (distance units)

Note that sigma is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum at $2^{1/6}\sigma$.

The last 2 coefficients are optional inner and outer cutoffs for style *lj/gromacs*. If not specified, the global *inner* and *outer* values are used.

The last 2 coefficients cannot be used with style *lj/gromacs/coul/gromacs* because this force field does not allow varying cutoffs for individual atom pairs; all pairs use the global cutoff(s) specified in the pair_style command.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/cut pair styles can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

None of the GROMACS pair styles support the *pair_modify* shift option, since the Lennard-Jones portion of the pair interaction is already smoothed to 0.0 at the cutoff.

The *pair_modify* table option is not relevant for this pair style.

None of the GROMACS pair styles support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure, since there are no corrections for a potential that goes to 0.0 at the cutoff.

All of the GROMACS pair styles write their information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

All of the GROMACS pair styles can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

18.230.4 Restrictions

none

18.230.5 Related commands

pair_coeff

Default: none

(Marrink) Marrink, de Vries, Mark, J Phys Chem B, 108, 750-760 (2004).

18.231 pair_style gw command

18.232 pair_style gw/zbl command

18.232.1 Syntax

```
pair_style style
```

- style = *gw* or *gw/zbl*

18.232.2 Examples

```
pair_style gw
pair_coeff * * SiC.gw Si C C

pair_style gw/zbl
pair_coeff * * SiC.gw.zbl C Si
```

18.232.3 Description

The *gw* style computes a 3-body *Gao-Weber* potential; similarly *gw/zbl* combines this potential with a modified repulsive ZBL core function in a similar fashion as implemented in the *tersoff/zbl* pair style.

Unfortunately the author of this contributed code has not been able to submit a suitable documentation explaining the details of the potentials. The LAMMPS developers thus have finally decided to release the code anyway with only the technical explanations. For details of the model and the parameters, please refer to the linked publication.

Only a single pair_coeff command is used with the *gw* and *gw/zbl* styles which specifies a Gao-Weber potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of GW elements to atom types

See the *pair_coeff* doc page for alternate ways to specify the path for the potential file.

As an example, imagine a file SiC.gw has Gao-Weber values for Si and C. If your LAMMPS simulation has 4 atoms types and you want the first 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * SiC.gw Si Si Si C
```

The first 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the GW file. The final C argument maps LAMMPS atom type 4 to the C element in the GW file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *gw* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Gao-Weber files in the *potentials* directory of the LAMMPS distribution have a ".gw" suffix. Gao-Weber with ZBL files have a ".gz.zbl" suffix. The structure of the potential files is similar to other many-body potentials supported by LAMMPS. You have to refer to the comments in the files and the literature to learn more details.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above from values in the potential file.

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.232.4 Restrictions

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This pair style requires the *newton* setting to be "on" for pair interactions.

The Gao-Weber potential files provided with LAMMPS (see the potentials directory) are parameterized for metal *units*. You can use the GW potential with any LAMMPS units, but you would need to create your own GW potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

18.232.5 Related commands

pair_coeff

Default: none

(Gao) Gao and Weber, Nuclear Instruments and Methods in Physics Research B 191 (2012) 504.

18.233 pair_style hbond/dreiding/lj command

18.234 pair_style hbond/dreiding/lj/omp command

18.235 pair_style hbond/dreiding/morse command

18.236 pair_style hbond/dreiding/morse/omp command

18.236.1 Syntax

```
pair_style style N inner_distance_cutoff outer_distance_cutoff angle_cutof
```

- style = *hbond/dreiding/lj* or *hbond/dreiding/morse*
- n = cosine angle periodicity
- inner_distance_cutoff = global inner cutoff for Donor-Acceptor interactions (distance units)
- outer_distance_cutoff = global cutoff for Donor-Acceptor interactions (distance units)
- angle_cutoff = global angle cutoff for Acceptor-Hydrogen-Donor
- interactions (degrees)

18.236.2 Examples

```
pair_style hybrid/overlay lj/cut 10.0 hbond/dreiding/lj 4 9.0 11.0 90
pair_coeff 1 2 hbond/dreiding/lj 3 i 9.5 2.75 4 9.0 11.0 90.0

pair_style hybrid/overlay lj/cut 10.0 hbond/dreiding/morse 2 9.0 11.0 90
pair_coeff 1 2 hbond/dreiding/morse 3 i 3.88 1.7241379 2.9 2 9 11 90
```

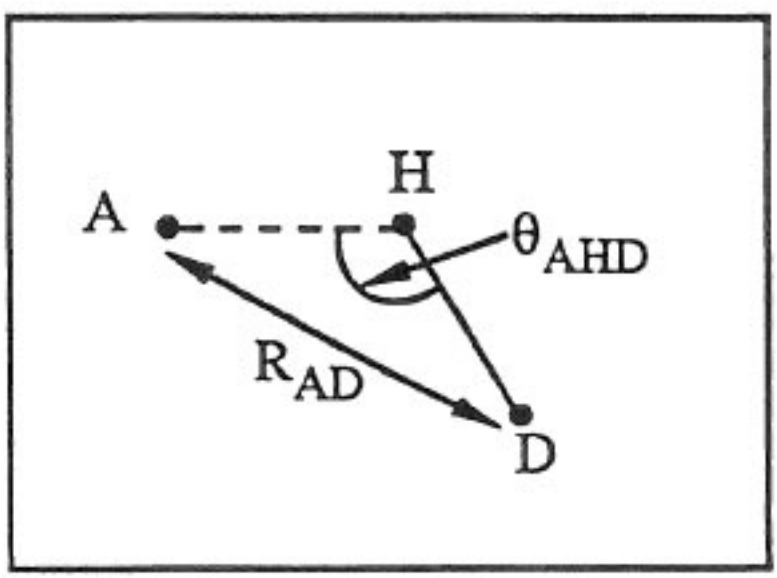
18.236.3 Description

The *hbond/dreiding* styles compute the Acceptor-Hydrogen-Donor (AHD) 3-body hydrogen bond interaction for the *DREIDING* force field, given by:

$$
\begin{aligned}
E =& [LJ(r)|Morse(r)] & r < r_{\mathrm{in}} \\
=& S(r) * [LJ(r)|Morse(r)] & r_{\mathrm{in}} < r < r_{\mathrm{out}} \\
=& 0 & r > r_{\mathrm{out}} \\
LJ(r) =& AR^{-12} - BR^{-10} cos^n\theta = \epsilon \left\{ 5 \left[\frac{\sigma}{r}\right]^{12} - 6 \left[\frac{\sigma}{r}\right]^{10} \right\} cos^n\theta \\
Morse(r) =& D_0 \left\{ \chi^2 - 2\chi \right\} cos^n\theta = D_0 \left\{ e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)} \right\} cos^n\theta \\
S(r) =& \frac{\left[r_{\mathrm{out}}^2 - r^2\right]^2 \left[r_{\mathrm{out}}^2 + 2r^2 - 3r_{\mathrm{in}}^2\right]}{\left[r_{\mathrm{out}}^2 - {r_{\mathrm{in}}}^2\right]^3}
\end{aligned}
$$

where r_{in} is the inner spline distance cutoff, r_{out} is the outer distance cutoff, θ_c is the angle cutoff, and *n* is the cosine periodicity.

Here, *r* is the radial distance between the donor (D) and acceptor (A) atoms and θ is the bond angle between the acceptor, the hydrogen (H) and the donor atoms:



These 3-body interactions can be defined for pairs of acceptor and donor atoms, based on atom types. For each donor/acceptor atom pair, the 3rd atom in the interaction is a hydrogen permanently bonded to the donor atom, e.g. in a bond list read in from a data file via the *read_data* command. The atom types of possible hydrogen atoms for each donor/acceptor type pair are specified by the *pair_coeff* command (see below).

Style *hbond/dreiding/lj* is the original DREIDING potential of *(Mayo)*. It uses a LJ 12/10 functional for the Donor-Acceptor interactions. To match the results in the original paper, use n = 4.

Style *hbond/dreiding/morse* is an improved version using a Morse potential for the Donor-Acceptor interactions. *(Liu)* showed that the Morse form gives improved results for Dendrimer simulations, when n = 2.

See the *Howto bioFF* doc page for more information on the DREIDING force field.

Note: Because the Dreiding hydrogen bond potential is only one portion of an overall force field which typically includes other pairwise interactions, it is common to use it as a sub-style in a *pair_style hybrid/overlay* command, where another pair style provides the repulsive core interaction between pairs of atoms, e.g. a 1/r^12 Lennard-Jones repulsion.

Note: When using the hbond/dreiding pair styles with *pair_style hybrid/overlay*, you should explicitly define pair interactions between the donor atom and acceptor atoms, (as well as between these atoms and ALL other atoms in your system). Whenever *pair_style hybrid/overlay* is used, ordinary mixing rules are not applied to atoms like the donor and acceptor atoms because they are typically referenced in multiple pair styles. Neglecting to do this can cause difficult-to-detect physics problems.

Note: In the original Dreiding force field paper 1-4 non-bonded interactions ARE allowed. If this is desired for your model, use the special_bonds command (e.g. "special_bonds lj 0.0 0.0 1.0") to turn these interactions on.

The following coefficients must be defined for pairs of eligible donor/acceptor types via the *pair_coeff* command as in the examples above.

Note: Unlike other pair styles and their associated *pair_coeff* commands, you do not need to specify pair_coeff settings for all possible I,J type pairs. Only I,J type pairs for atoms which act as joint donors/acceptors need to be specified; all other type pairs are assumed to be inactive.

Note: A *pair_coeff* command can be specified multiple times for the same donor/acceptor type pair. This enables multiple hydrogen types to be assigned to the same donor/acceptor type pair. For other pair_styles, if the pair_coeff command is re-used for the same I,J type pair, the settings for that type pair are overwritten. For the hydrogen bond potentials this is not the case; the settings are cumulative. This means the only way to turn off a previous setting, is to re-use the pair_style command and start over.

For the *hbond/dreiding/lj* style the list of coefficients is as follows:

- K = hydrogen atom type = 1 to Ntypes
- donor flag = *i* or *j*
- ϵ (energy units)
- σ (distance units)
- n = exponent in formula above
- distance cutoff r_{in} (distance units)
- distance cutoff r_{out} (distance units)

- angle cutoff (degrees)

For the *hbond/dreiding/morse* style the list of coefficients is as follows:

- K = hydrogen atom type = 1 to Ntypes
- donor flag = *i* or *j*
- D_0 (energy units)
- α (1/distance units)
- r_0 (distance units)
- *n* = exponent in formula above
- distance cutoff r_{in} (distance units)
- distance cutoff r_{out} (distance units)
- angle cutoff (degrees)

A single hydrogen atom type K can be specified, or a wild-card asterisk can be used in place of or in conjunction with the K arguments to select multiple types as hydrogen atoms. This takes the form "*" or "*n" or "n*" or "m*n". See the *pair_coeff* command doc page for details.

If the donor flag is *i*, then the atom of type I in the pair_coeff command is treated as the donor, and J is the acceptor. If the donor flag is *j*, then the atom of type J in the pair_coeff command is treated as the donor and I is the donor. This option is required because the *pair_coeff* command requires that I <= J.

ϵ and σ are settings for the hydrogen bond potential based on a Lennard-Jones functional form. Note that sigma is defined as the zero-crossing distance for the potential, not as the energy minimum at $2^{1/6}\sigma$.

D_0 and α and r_0 are settings for the hydrogen bond potential based on a Morse functional form.

The last 3 coefficients for both styles are optional. If not specified, the global n, distance cutoff, and angle cutoff specified in the pair_style command are used. If you wish to only override the 2nd or 3rd optional parameter, you must also specify the preceding optional parameters.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support mixing. You must explicitly identify each donor/acceptor type pair.

These styles do not support the *pair_modify* shift option for the energy of the interactions.

The *pair_modify* table option is not relevant for these pair styles.

These pair styles do not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

These pair styles do not write their information to *binary restart files*, so pair_style and pair_coeff commands need to be re-specified in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

These pair styles tally a count of how many hydrogen bonding interactions they calculate each timestep and the hbond energy. These quantities can be accessed via the *compute pair* command as a vector of values of length 2.

To print these quantities to the log file (with a descriptive column heading) the following commands could be included in an input script:

```
compute hb all pair hbond/dreiding/lj
variable n_hbond equal c_hb[1] #number hbonds
variable E_hbond equal c_hb[2] #hbond energy
thermo_style custom step temp epair v_E_hbond
```

18.236.4 Restrictions

none

18.236.5 Related commands

pair_coeff

Default: none

(Mayo) Mayo, Olfason, Goddard III, J Phys Chem, 94, 8897-8909 (1990).

(Liu) Liu, Bryantsev, Diallo, Goddard III, J. Am. Chem. Soc 131 (8) 2798 (2009)

18.237 pair_style hybrid command

18.238 pair_style hybrid/kk command

18.239 pair_style hybrid/overlay command

18.240 pair_style hybrid/overlay/kk command

18.240.1 Syntax

```
pair_style hybrid style1 args style2 args ...
pair_style hybrid/overlay style1 args style2 args ...
```

- style1,style2 = list of one or more pair styles and their arguments

18.240.2 Examples

```
pair_style hybrid lj/cut/coul/cut 10.0 eam lj/cut 5.0
pair_coeff 1*2 1*2 eam niu3
pair_coeff 3 3 lj/cut/coul/cut 1.0 1.0
pair_coeff 1*2 3 lj/cut 0.5 1.2

pair_style hybrid/overlay lj/cut 2.5 coul/long 2.0
pair_coeff * * lj/cut 1.0 1.0
pair_coeff * * coul/long
```

18.240.3 Description

The *hybrid* and *hybrid/overlay* styles enable the use of multiple pair styles in one simulation. With the *hybrid* style, exactly one pair style is assigned to each pair of atom types. With the *hybrid/overlay* style, one or more pair styles can be assigned to each pair of atom types. The assignment of pair styles to type pairs is made via the *pair_coeff* command.

Here are two examples of hybrid simulations. The *hybrid* style could be used for a simulation of a metal droplet on a LJ surface. The metal atoms interact with each other via an *eam* potential, the surface atoms interact with each other via a *lj/cut* potential, and the metal/surface interaction is also computed via a *lj/cut* potential. The *hybrid/overlay* style could be used as in the 2nd example above, where multiple potentials are superposed in an additive fashion to compute the interaction between atoms. In this example, using *lj/cut* and *coul/long* together gives the same result as if the *lj/cut/coul/long* potential were used by itself. In this case, it would be more efficient to use the single combined potential, but in general any combination of pair potentials can be used together in to produce an interaction that is not encoded in any single pair_style file, e.g. adding Coulombic forces between granular particles.

All pair styles that will be used are listed as "sub-styles" following the *hybrid* or *hybrid/overlay* keyword, in any order. Each sub-style's name is followed by its usual arguments, as illustrated in the example above. See the doc pages of individual pair styles for a listing and explanation of the appropriate arguments.

Note that an individual pair style can be used multiple times as a sub-style. For efficiency this should only be done if your model requires it. E.g. if you have different regions of Si and C atoms and wish to use a Tersoff potential for pure Si for one set of atoms, and a Tersoff potential for pure C for the other set (presumably with some 3rd potential for Si-C interactions), then the sub-style *tersoff* could be listed twice. But if you just want to use a Lennard-Jones or other pairwise potential for several different atom type pairs in your model, then you should just list the sub-style once and use the pair_coeff command to assign parameters for the different type pairs.

Note: There is one exception to this option to list an individual pair style multiple times: GPU-enabled pair styles in the GPU package. This is because the GPU package currently assumes that only one instance of a pair style is being used.

In the pair_coeff commands, the name of a pair style must be added after the I,J type specification, with the remaining coefficients being those appropriate to that style. If the pair style is used multiple times in the pair_style command, then an additional numeric argument must also be specified which is a number from 1 to M where M is the number of times the sub-style was listed in the pair style command. The extra number indicates which instance of the sub-style these coefficients apply to.

For example, consider a simulation with 3 atom types: types 1 and 2 are Ni atoms, type 3 are LJ atoms with charges. The following commands would set up a hybrid simulation:

```
pair_style hybrid eam/alloy lj/cut/coul/cut 10.0 lj/cut 8.0
pair_coeff * * eam/alloy nialhjea Ni Ni NULL
```

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```
pair_coeff 3 3 lj/cut/coul/cut 1.0 1.0
pair_coeff 1*2 3 lj/cut 0.8 1.3
```

As an example of using the same pair style multiple times, consider a simulation with 2 atom types. Type 1 is Si, type 2 is C. The following commands would model the Si atoms with Tersoff, the C atoms with Tersoff, and the cross-interactions with Lennard-Jones:

```
pair_style hybrid lj/cut 2.5 tersoff tersoff
pair_coeff * * tersoff 1 Si.tersoff Si NULL
pair_coeff * * tersoff 2 C.tersoff NULL C
pair_coeff 1 2 lj/cut 1.0 1.5
```

If pair coefficients are specified in the data file read via the *read_data* command, then the same rule applies. E.g. "eam/alloy" or "lj/cut" must be added after the atom type, for each line in the "Pair Coeffs" section, e.g.

```
Pair Coeffs

1 lj/cut/coul/cut 1.0 1.0
...
```

Note that the pair_coeff command for some potentials such as *pair_style eam/alloy* includes a mapping specification of elements to all atom types, which in the hybrid case, can include atom types not assigned to the *eam/alloy* potential. The NULL keyword is used by many such potentials (eam/alloy, Tersoff, AIREBO, etc), to denote an atom type that will be assigned to a different sub-style.

For the *hybrid* style, each atom type pair I,J is assigned to exactly one sub-style. Just as with a simulation using a single pair style, if you specify the same atom type pair in a second pair_coeff command, the previous assignment will be overwritten.

For the *hybrid/overlay* style, each atom type pair I,J can be assigned to one or more sub-styles. If you specify the same atom type pair in a second pair_coeff command with a new sub-style, then the second sub-style is added to the list of potentials that will be calculated for two interacting atoms of those types. If you specify the same atom type pair in a second pair_coeff command with a sub-style that has already been defined for that pair of atoms, then the new pair coefficients simply override the previous ones, as in the normal usage of the pair_coeff command. E.g. these two sets of commands are the same:

```
pair_style lj/cut 2.5
pair_coeff * * 1.0 1.0
pair_coeff 2 2 1.5 0.8

pair_style hybrid/overlay lj/cut 2.5
pair_coeff * * lj/cut 1.0 1.0
pair_coeff 2 2 lj/cut 1.5 0.8
```

Coefficients must be defined for each pair of atoms types via the *pair_coeff* command as described above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below.

For both the *hybrid* and *hybrid/overlay* styles, every atom type pair I,J (where I <= J) must be assigned to at least one sub-style via the *pair_coeff* command as in the examples above, or in the data file read by the *read_data*, or by mixing as described below.

If you want there to be no interactions between a particular pair of atom types, you have 3 choices. You can assign the type pair to some sub-style and use the *neigh_modify exclude type* command. You can assign it to some sub-style and set the coefficients so that there is effectively no interaction (e.g. epsilon = 0.0 in a LJ potential). Or, for *hybrid* and *hybrid/overlay* simulations, you can use this form of the pair_coeff command in your input script:

```
pair_coeff        2 3 none
```

or this form in the "Pair Coeffs" section of the data file:

```
3 none
```

If an assignment to *none* is made in a simulation with the *hybrid/overlay* pair style, it wipes out all previous assignments of that atom type pair to sub-styles.

Note that you may need to use an *atom_style* hybrid command in your input script, if atoms in the simulation will need attributes from several atom styles, due to using multiple pair potentials.

Different force fields (e.g. CHARMM vs AMBER) may have different rules for applying weightings that change the strength of pairwise interactions between pairs of atoms that are also 1-2, 1-3, and 1-4 neighbors in the molecular bond topology, as normally set by the *special_bonds* command. Different weights can be assigned to different pair hybrid sub-styles via the *pair_modify special* command. This allows multiple force fields to be used in a model of a hybrid system, however, there is no consistent approach to determine parameters automatically for the interactions between the two force fields, this is only recommended when particles described by the different force fields do not mix.

Here is an example for mixing CHARMM and AMBER: The global *amber* setting sets the 1-4 interactions to non-zero scaling factors and then overrides them with 0.0 only for CHARMM:

```
special_bonds amber
pair_hybrid lj/charmm/coul/long 8.0 10.0 lj/cut/coul/long 10.0
pair_modify pair lj/charmm/coul/long special lj/coul 0.0 0.0 0.0
```

The this input achieves the same effect:

```
special_bonds 0.0 0.0 0.1
pair_hybrid lj/charmm/coul/long 8.0 10.0 lj/cut/coul/long 10.0
pair_modify pair lj/cut/coul/long special lj 0.0 0.0 0.5
pair_modify pair lj/cut/coul/long special coul 0.0 0.0 0.83333333
pair_modify pair lj/charmm/coul/long special lj/coul 0.0 0.0 0.0
```

Here is an example for mixing Tersoff with OPLS/AA based on a data file that defines bonds for all atoms where for the Tersoff part of the system the force constants for the bonded interactions have been set to 0. Note the global settings are effectively *lj/coul 0.0 0.0 0.5* as required for OPLS/AA:

```
special_bonds lj/coul 1e-20 1e-20 0.5
pair_hybrid tersoff lj/cut/coul/long 12.0
pair_modify pair tersoff special lj/coul 1.0 1.0 1.0
```

For use with the various *compute */tally* computes, the *pair_modify compute/tally* command can be used to selectively turn off processing of the compute tally styles, for example, if those pair styles (e.g. many-body styles) do not support this feature.

See the *pair_modify* doc page for details on the specific syntax, requirements and restrictions.

The potential energy contribution to the overall system due to an individual sub-style can be accessed and output via the *compute pair* command.

Note: Several of the potentials defined via the pair_style command in LAMMPS are really many-body potentials, such as Tersoff, AIREBO, MEAM, ReaxFF, etc. The way to think about using these potentials in a hybrid setting is as follows.

A subset of atom types is assigned to the many-body potential with a single *pair_coeff* command, using "* *" to include all types and the NULL keywords described above to exclude specific types not assigned to that potential. If types 1,3,4 were assigned in that way (but not type 2), this means that all many-body interactions between all atoms of types 1,3,4 will be computed by that potential. Pair_style hybrid allows interactions between type pairs 2-2, 1-2, 2-3, 2-4 to be specified for computation by other pair styles. You could even add a second interaction for 1-1 to be computed by another pair style, assuming pair_style hybrid/overlay is used.

But you should not, as a general rule, attempt to exclude the many-body interactions for some subset of the type pairs within the set of 1,3,4 interactions, e.g. exclude 1-1 or 1-3 interactions. That is not conceptually well-defined for many-body interactions, since the potential will typically calculate energies and foces for small groups of atoms, e.g. 3 or 4 atoms, using the neighbor lists of the atoms to find the additional atoms in the group. It is typically non-physical to think of excluding an interaction between a particular pair of atoms when the potential computes 3-body or 4-body interactions.

However, you can still use the pair_coeff none setting or the *neigh_modify exclude* command to exclude certain type pairs from the neighbor list that will be passed to a many-body sub-style. This will alter the calculations made by a many-body potential, since it builds its list of 3-body, 4-body, etc interactions from the pair list. You will need to think carefully as to whether it produces a physically meaningful result for your model.

For example, imagine you have two atom types in your model, type 1 for atoms in one surface, and type 2 for atoms in the other, and you wish to use a Tersoff potential to compute interactions within each surface, but not between surfaces. Then either of these two command sequences would implement that model:

```
pair_style hybrid tersoff
pair_coeff * * tersoff SiC.tersoff C C
pair_coeff 1 2 none

pair_style tersoff
pair_coeff * * SiC.tersoff C C
neigh_modify exclude type 1 2
```

Either way, only neighbor lists with 1-1 or 2-2 interactions would be passed to the Tersoff potential, which means it would compute no 3-body interactions containing both type 1 and 2 atoms.

Here is another example, using hybrid/overlay, to use 2 many-body potentials together, in an overlapping manner. Imagine you have CNT (C atoms) on a Si surface. You want to use Tersoff for Si/Si and Si/C interactions, and AIREBO for C/C interactions. Si atoms are type 1; C atoms are type 2. Something like this will work:

```
pair_style hybrid/overlay tersoff airebo 3.0
pair_coeff * * tersoff SiC.tersoff.custom Si C
pair_coeff * * airebo CH.airebo NULL C
```

Note that to prevent the Tersoff potential from computing C/C interactions, you would need to modify the SiC.tersoff file to turn off C/C interaction, i.e. by setting the appropriate coefficients to 0.0.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page.

Since the *hybrid* and *hybrid/overlay* styles delegate computation to the individual sub-styles, the suffix versions of the *hybrid* and *hybrid/overlay* styles are used to propagate the corresponding suffix to all sub-styles, if those versions exist. Otherwise the non-accelerated version will be used.

The individual accelerated sub-styles are part of the GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

Any pair potential settings made via the *pair_modify* command are passed along to all sub-styles of the hybrid potential.

For atom type pairs I,J and I != J, if the sub-style assigned to I,I and J,J is the same, and if the sub-style allows for mixing, then the coefficients for I,J can be mixed. This means you do not have to specify a pair_coeff command for I,J since the I,J type pair will be assigned automatically to the sub-style defined for both I,I and J,J and its coefficients generated by the mixing rule used by that sub-style. For the *hybrid/overlay* style, there is an additional requirement that both the I,I and J,J pairs are assigned to a single sub-style. See the "pair_modify" command for details of mixing rules. See the See the doc page for the sub-style to see if allows for mixing.

The hybrid pair styles supports the *pair_modify* shift, table, and tail options for an I,J pair interaction, if the associated sub-style supports it.

For the hybrid pair styles, the list of sub-styles and their respective settings are written to *binary restart files*, so a *pair_style* command does not need to specified in an input script that reads a restart file. However, the coefficient information is not stored in the restart file. Thus, pair_coeff commands need to be re-specified in the restart input script.

These pair styles support the use of the *inner*, *middle*, and *outer* keywords of the *run_style respa* command, if their sub-styles do.

18.240.4 Restrictions

When using a long-range Coulombic solver (via the *kspace_style* command) with a hybrid pair_style, one or more sub-styles will be of the "long" variety, e.g. *lj/cut/coul/long* or *buck/coul/long*. You must insure that the short-range Coulombic cutoff used by each of these long pair styles is the same or else LAMMPS will generate an error.

18.240.5 Related commands

pair_coeff

Default: none

18.241 pair_style ilp/graphene/hbn command

18.241.1 Syntax

```
pair_style [hybrid/overlay ...] ilp/graphene/hbn cutoff tap_flag
```

- cutoff = global cutoff (distance units)
- tap_flag = 0/1 to turn off/on the taper function

18.241.2 Examples

```
pair_style  hybrid/overlay ilp/graphene/hbn 16.0 1
pair_coeff  * * ilp/graphene/hbn  BNCH.ILP B N C

pair_style  hybrid/overlay rebo tersoff ilp/graphene/hbn 16.0 coul/shield 16.0
pair_coeff  * * rebo              CH.rebo     NULL NULL C
pair_coeff  * * tersoff           BNC.tersoff B    N    NULL
pair_coeff  * * ilp/graphene/hbn  BNCH.ILP    B    N    C
pair_coeff  1 1 coul/shield 0.70
pair_coeff  1 2 coul/shield 0.695
pair_coeff  2 2 coul/shield 0.69
```

18.241.3 Description

The *ilp/graphene/hbn* style computes the registry-dependent interlayer potential (ILP) potential as described in *(Leven1)*, *(Leven2)* and *(Maaravi)*. The normals are calculated in the way as described in *(Kolmogorov)*.

$$
\begin{aligned}
E =& \frac{1}{2}\sum_i \sum_{j\neq i} V_{ij} \\
V_{ij} =& \mathrm{Tap}(r_{ij}) \left\{ e^{-\alpha(r_{ij}/\beta-1)} \left[\epsilon + f(\rho_{ij}) + f(\rho_{ji})\right] - \frac{1}{1+e^{-d[(r_{ij}/(s_R\cdot r^{eff}))-1]}} \cdot \frac{C_6}{r_{ij}^6} \right\} \\
\rho_{ij}^2 =& r_{ij}^2 - (\mathbf{r}_{ij}\cdot\mathbf{n}_i)^2 \\
\rho_{ji}^2 =& r_{ij}^2 - (\mathbf{r}_{ij}\cdot\mathbf{n}_j)^2 \\
f(\rho) =& Ce^{-(\rho/\delta)^2} \\
\mathrm{Tap}(r_{ij}) =& 20\left(\frac{r_{ij}}{R_{cut}}\right)^7 - 70\left(\frac{r_{ij}}{R_{cut}}\right)^6 + 84\left(\frac{r_{ij}}{R_{cut}}\right)^5 - 35\left(\frac{r_{ij}}{R_{cut}}\right)^4 + 1
\end{aligned}
$$

Where $\mathrm{Tap}(r_{ij})$ is the taper function which provides a continuous cutoff (up to third derivative) for interatomic separations larger than r_c *(Maaravi)*. The definitions of each parameter in the above equation can be found in *(Leven1)* and *(Maaravi)*.

It is important to include all the pairs to build the neighbor list for calculating the normals.

Note: This potential (ILP) is intended for interlayer interactions between two different layers of graphene, hexagonal boron nitride (h-BN) and their hetero-junction. To perform a realistic simulation, this potential must be used in combination with intralayer potential, such as *AIREBO* or *Tersoff* potential. To keep the intralayer properties unaffected, the interlayer interaction within the same layers should be avoided. Hence, each atom has to have a layer identifier such that atoms residing on the same layer interact via the appropriate intralayer potential and atoms residing on different layers interact via the ILP. Here, the molecule id is chosen as the layer identifier, thus a data file with the "full" atom style is required to use this potential.

The parameter file (e.g. BNCH.ILP), is intended for use with *metal* *units*, with energies in meV. Two additional parameters, *S*, and *rcut* are included in the parameter file. *S* is designed to facilitate scaling of energies. *rcut* is designed to build the neighbor list for calculating the normals for each atom pair.

Note: The parameters presented in the parameter file (e.g. BNCH.ILP), are fitted with taper function by setting the cutoff equal to 16.0 Angstrom. Using different cutoff or taper function should be careful. The parameters for atoms

pairs between Boron and Nitrogen are fitted with a screened Coulomb interaction *coul/shield*. Therefore, to simulated the properties of h-BN correctly, this potential must be used in combination with the pair style *coul/shield*.

Note: Four new sets of parameters of ILP for 2D layered Materials with bilayer and bulk configurations are presented in *(Ouyang1)* and *(Ouyang2)*, respectively. These parameters provide a good description in both short- and long-range interaction regimes. While the old ILP parameters published in *(Leven2)* and *(Maaravi)* are only suitable for long-range interaction regime. This feature is essential for simulations in high pressure regime (i.e., the interlayer distance is smaller than the equilibrium distance). The benchmark tests and comparison of these parameters can be found in *(Ouyang1)* and *(Ouyang2)*.

This potential must be used in combination with hybrid/overlay. Other interactions can be set to zero using pair_style *none*.

This pair style tallies a breakdown of the total interlayer potential energy into sub-categories, which can be accessed via the *compute pair* command as a vector of values of length 2. The 2 values correspond to the following sub-categories:

1. *E_vdW* = vdW (attractive) energy
2. *E_Rep* = Repulsive energy

To print these quantities to the log file (with descriptive column headings) the following commands could be included in an input script:

```
compute 0 all pair ilp/graphene/hbn
variable Evdw  equal c_0[1]
variable Erep  equal c_0[2]
thermo_style custom step temp epair v_Erep v_Evdw
```

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the pair_modify mix, shift, table, and tail options.

This pair style does not write their information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

18.241.4 Restrictions

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This pair potential requires the newton setting to be *on* for pair interactions.

The BNCH.ILP potential file provided with LAMMPS (see the potentials directory) are parameterized for *metal* units. You can use this potential with any LAMMPS units, but you would need to create your BNCH.ILP potential file with coefficients listed in the appropriate units, if your simulation does not use *metal* units.

18.241.5 Related commands

pair_coeff, *pair_none*, *pair_style hybrid/overlay*, *pair_style drip*, *pair_style pair_kolmogorov_crespi_z*, *pair_style pair_kolmogorov_crespi_full*, *pair_style pair_lebedeva_z*, *pair_style pair_coul_shield*.

Default: tap_flag = 1

(Leven1) I. Leven, I. Azuri, L. Kronik and O. Hod, J. Chem. Phys. 140, 104106 (2014).

(Leven2) I. Leven et al, J. Chem.Theory Comput. 12, 2896-905 (2016).

(Maaravi) T. Maaravi et al, J. Phys. Chem. C 121, 22826-22835 (2017).

(Kolmogorov) A. N. Kolmogorov, V. H. Crespi, Phys. Rev. B 71, 235415 (2005).

(Ouyang1) W. Ouyang, D. Mandelli, M. Urbakh and O. Hod, Nano Lett. 18, 6009-6016 (2018).

(Ouyang2) W. Ouyang et al., J. Chem. Theory Comput. 16(1), 666-676 (2020).

18.242 pair_style kim command

18.242.1 Syntax

```
pair_style kim model
```

model = name of a KIM model (the KIM ID for models archived in OpenKIM)

18.242.2 Examples

```
pair_style kim SW_StillingerWeber_1985_Si__MO_405512056662_005
pair_coeff * * Si
```

18.242.3 Description

This pair style is a wrapper on the Open Knowledgebase of Interatomic Models (OpenKIM) repository of interatomic potentials to enable their use in LAMMPS scripts.

The preferred interface for using interatomic models archived in OpenKIM is the *kim_commands interface*. That interface supports both "KIM Portable Models" (PMs) that conform to the KIM API Portable Model Interface (PMI) and can be used by any simulation code that conforms to the KIM API/PMI, and "KIM Simulator Models" that are natively implemented within a single simulation code (like LAMMPS) and can only be used with it. The *pair_style kim* command is limited to KIM PMs. It is used by the *kim_commands interface* as needed.

Note: Since *pair_style kim* is called by *kim_interactions* as needed, is not recommended to be directly used in input scripts.

The argument *model* is the name of the KIM PM. For potentials archived in OpenKIM this is the extended KIM ID (see *kim_commands* for details). LAMMPS can invoke any KIM PM, however there can be incompatibilities (for example

due to unit matching issues). In the event of an incompatibility, the code will terminate with an error message. Check both the LAMMPS and KIM log files for details.

Only a single *pair_coeff* command is used with the *kim* style, which specifies the mapping of LAMMPS atom types to the species supported by the KIM PM. This is done by specifying *N* additional arguments after the * * in the *pair_coeff* command, where *N* is the number of LAMMPS atom types:

- N element names = mapping of KIM elements to atom types

For example, consider a KIM PM that supports Si and C species. If the LAMMPS simulation has four atom types, where the first three are Si, and the fourth is C, the following *pair_coeff* command would be used:

```
pair_coeff * * Si Si Si C
```

The first two arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1, 2, and 3 to Si as defined within KIM PM. The final C argument maps LAMMPS atom type 4 to C.

In addition to the usual LAMMPS error messages, the KIM library itself may generate errors, which should be printed to the screen. In this case it is also useful to check the *kim.log* file for additional error information. The file *kim.log* should be generated in the same directory where LAMMPS is running.

To download, build, and install the KIM library on your system, see the *lib/kim/README* file. Once you have done this and built LAMMPS with the KIM package installed you can run the example input scripts in *examples/kim*.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the *pair_modify* mix, shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since KIM stores the potential parameters. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.242.4 Restrictions

This pair style is part of the KIM package. See details on restrictions in *kim_commands*.

This current version of pair_style kim is compatible with the kim-api package version 2.0.0 and higher.

18.242.5 Related commands

pair_coeff, *kim_commands*

Default: none

18.243 pair_style kolmogorov/crespi/full command

18.243.1 Syntax

```
pair_style hybrid/overlay kolmogorov/crespi/full cutoff tap_flag
```

- cutoff = global cutoff (distance units)
- tap_flag = 0/1 to turn off/on the taper function

18.243.2 Examples

```
pair_style hybrid/overlay kolmogorov/crespi/full 20.0 0
pair_coeff * * none
pair_coeff * * kolmogorov/crespi/full  CH.KC   C C

pair_style hybrid/overlay rebo kolmogorov/crespi/full 16.0 1
pair_coeff * * rebo                    CH.rebo      C H
pair_coeff * * kolmogorov/crespi/full  CH_taper.KC  C H
```

18.243.3 Description

The *kolmogorov/crespi/full* style computes the Kolmogorov-Crespi (KC) interaction potential as described in *(Kolmogorov)*. No simplification is made,

$$
\begin{aligned}
E =& \frac{1}{2}\sum_i \sum_{j\neq i} V_{ij} \\
V_{ij} =& e^{-\lambda(r_{ij}-z_0)}\left[C + f(\rho_{ij}) + f(\rho_{ji}) - A\left(\frac{r_{ij}}{z_0}\right)^{-6}\right] \\
\rho_{ij}^2 =& r_{ij}^2 - (\mathbf{r}_{ij}\cdot\mathbf{n}_i)^2 \\
\rho_{ji}^2 =& r_{ij}^2 - (\mathbf{r}_{ij}\cdot\mathbf{n}_j)^2 \\
f(\rho) =& e^{-(\rho/\delta)^2}\sum_{n=0}^{2} C_{2n}(\rho/\delta)^{2n}
\end{aligned}
$$

It is important to have a sufficiently large cutoff to ensure smooth forces and to include all the pairs to build the neighbor list for calculating the normals. Energies are shifted so that they go continuously to zero at the cutoff assuming that the exponential part of V_{ij} (first term) decays sufficiently fast. This shift is achieved by the last term in the equation for V_{ij} above. This is essential only when the tapper function is turned off. The formula of taper function can be found in pair style *ilp/graphene/hbn*.

Note: This potential (ILP) is intended for interlayer interactions between two different layers of graphene. To perform a realistic simulation, this potential must be used in combination with intralayer potential, such as *AIREBO* or *Tersoff* potential. To keep the intralayer properties unaffected, the interlayer interaction within the same layers should be avoided. Hence, each atom has to have a layer identifier such that atoms residing on the same layer interact via the appropriate intralayer potential and atoms residing on different layers interact via the ILP. Here, the molecule id is chosen as the layer identifier, thus a data file with the "full" atom style is required to use this potential.

The parameter file (e.g. CH.KC), is intended for use with *metal units*, with energies in meV. Two additional parameters, *S*, and *rcut* are included in the parameter file. *S* is designed to facilitate scaling of energies. *rcut* is designed to build the neighbor list for calculating the normals for each atom pair.

Note: Two new sets of parameters of KC potential for hydrocarbons, CH.KC (without the taper function) and CH_taper.KC (with the taper function) are presented in *(Ouyang1)*. The energy for the KC potential with the taper function goes continuously to zero at the cutoff. The parameters in both CH.KC and CH_taper.KC provide a good description in both short- and long-range interaction regimes. While the original parameters (CC.KC) published in *(Kolmogorov)* are only suitable for long-range interaction regime. This feature is essential for simulations in high pressure regime (i.e., the interlayer distance is smaller than the equilibrium distance). The benchmark tests and comparison of these parameters can be found in *(Ouyang1)* and *(Ouyang2)*.

This potential must be used in combination with hybrid/overlay. Other interactions can be set to zero using pair_style *none*.

This pair style tallies a breakdown of the total interlayer potential energy into sub-categories, which can be accessed via the *compute pair* command as a vector of values of length 2. The 2 values correspond to the following sub-categories:

1. *E_vdW* = vdW (attractive) energy
2. *E_Rep* = Repulsive energy

To print these quantities to the log file (with descriptive column headings) the following commands could be included in an input script:

```
compute 0 all pair kolmogorov/crespi/full
variable Evdw  equal c_0[1]
variable Erep  equal c_0[2]
thermo_style custom step temp epair v_Erep v_Evdw
```

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the pair_modify mix, shift, table, and tail options.

This pair style does not write their information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

18.243.4 Restrictions

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This pair potential requires the newton setting to be *on* for pair interactions.

The CH.KC potential file provided with LAMMPS (see the potentials folder) are parameterized for metal units. You can use this potential with any LAMMPS units, but you would need to create your own custom CC.KC potential file with all coefficients converted to the appropriate units.

18.243.5 Related commands

pair_coeff, *pair_none*, *pair_style hybrid/overlay*, *pair_style drip*, *pair_style pair_lebedeva_z*, *pair_style kolmogorov/crespi/z*, *pair_style ilp/graphene/hbn*.

Default: tap_flag = 0

(Kolmogorov) A. N. Kolmogorov, V. H. Crespi, Phys. Rev. B 71, 235415 (2005)

(Ouyang1) W. Ouyang, D. Mandelli, M. Urbakh and O. Hod, Nano Lett. 18, 6009-6016 (2018).

(Ouyang2) W. Ouyang et al., J. Chem. Theory Comput. 16(1), 666-676 (2020).

18.244 pair_style kolmogorov/crespi/z command

18.244.1 Syntax

```
pair_style [hybrid/overlay ...] kolmogorov/crespi/z cutoff
```

18.244.2 Examples

```
pair_style hybrid/overlay kolmogorov/crespi/z 20.0
pair_coeff * * none
pair_coeff 1 2 kolmogorov/crespi/z  CC.KC   C C

pair_style hybrid/overlay rebo kolmogorov/crespi/z 14.0
pair_coeff * * rebo                 CH.rebo    C C
pair_coeff 1 2 kolmogorov/crespi/z  CC.KC      C C
```

18.244.3 Description

The *kolmogorov/crespi/z* style computes the Kolmogorov-Crespi interaction potential as described in *(Kolmogorov)*. An important simplification is made, which is to take all normals along the z-axis.

$$
\begin{aligned}
E =& \frac{1}{2} \sum_i \sum_{j \neq i} V_{ij} \\
V_{ij} =& e^{-\lambda(r_{ij} - z_0)} \left[C + f(\rho_{ij}) + f(\rho_{ji})\right] - A \left(\frac{r_{ij}}{z_0}\right)^{-6} + A \left(\frac{\text{cutoff}}{z_0}\right)^{-6} \\
\rho_{ij}^2 =& \rho_{ji}^2 = x_{ij}^2 + y_{ij}^2 \qquad\qquad (\mathbf{n}_i \equiv \hat{\mathbf{z}}) \\
f(\rho) =& e^{-(\rho/\delta)^2} \sum_{n=0}^{2} C_{2n} \left(\rho/\delta\right)^{2n}
\end{aligned}
$$

It is important to have a sufficiently large cutoff to ensure smooth forces. Energies are shifted so that they go continuously to zero at the cutoff assuming that the exponential part of V_{ij} (first term) decays sufficiently fast. This shift is achieved by the last term in the equation for V_{ij} above.

This potential is intended for interactions between two layers of graphene. Therefore, to avoid interaction between layers in multi-layered materials, each layer should have a separate atom type and interactions should only be computed between atom types of neighboring layers.

The parameter file (e.g. CC.KC), is intended for use with metal *units*, with energies in meV. An additional parameter, *S*, is available to facilitate scaling of energies in accordance with *(vanWijk)*.

This potential must be used in combination with hybrid/overlay. Other interactions can be set to zero using pair_style *none*.

18.244.4 Restrictions

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.244.5 Related commands

pair_coeff, *pair_none*, *pair_style hybrid/overlay*, *pair_style drip*, *pair_style ilp/graphene/hbn*. *pair_style kolmogorov/crespi/full*, *pair_style lebedeva/z*

Default: none

(Kolmogorov) A. N. Kolmogorov, V. H. Crespi, Phys. Rev. B 71, 235415 (2005)

(vanWijk) M. M. van Wijk, A. Schuring, M. I. Katsnelson, and A. Fasolino, Physical Review Letters, 113, 135504 (2014)

18.245 pair_style lcbop command

18.245.1 Syntax

```
pair_style lcbop
```

18.245.2 Examples

```
pair_style lcbop
pair_coeff * * ../potentials/C.lcbop C
```

18.245.3 Description

The *lcbop* pair style computes the long-range bond-order potential for carbon (LCBOP) of *(Los and Fasolino)*. See section II in that paper for the analytic equations associated with the potential.

Only a single pair_coeff command is used with the *lcbop* style which specifies an LCBOP potential file with parameters for specific elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of LCBOP elements to atom types

See the *pair_coeff* doc page for alternate ways to specify the path for the potential file.

As an example, if your LAMMPS simulation has 4 atom types and you want the 1st 3 to be C you would use the following pair_coeff command:

```
pair_coeff * * C.lcbop C C C NULL
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first C argument maps LAMMPS atom type 1 to the C element in the LCBOP file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *lcbop* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

The parameters/coefficients for the LCBOP potential as applied to C are listed in the C.lcbop file to agree with the original *(Los and Fasolino)* paper. Thus the parameters are specific to this potential and the way it was fit, so modifying the file should be done carefully.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the *pair_modify* mix, shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.245.4 Restrictions

This pair styles is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This pair potential requires the *newton* setting to be "on" for pair interactions.

The C.lcbop potential file provided with LAMMPS (see the potentials directory) is parameterized for metal *units*. You can use the LCBOP potential with any LAMMPS units, but you would need to create your own LCBOP potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

18.245.5 Related commands

pair_airebo, *pair_coeff*

Default: none

(Los and Fasolino) J. H. Los and A. Fasolino, Phys. Rev. B 68, 024107 (2003).

18.246 pair_style lebedeva/z command

18.246.1 Syntax

```
pair_style [hybrid/overlay ...] lebedeva/z cutoff
```

18.246.2 Examples

```
pair_style hybrid/overlay lebedeva/z 20.0
pair_coeff * * none
pair_coeff 1 2 lebedeva/z  CC.Lebedeva   C C

pair_style hybrid/overlay rebo lebedeva/z 14.0
pair_coeff * * rebo        CH.rebo       C C
pair_coeff 1 2 lebedeva/z  CC.Lebedeva   C C
```

18.246.3 Description

The *lebedeva/z* style computes the Lebedeva interaction potential as described in *(Lebedeva et al.)*. An important simplification is made, which is to take all normals along the z-axis.

$$
\begin{aligned}
E =& \frac{1}{2}\sum_i \sum_{i\neq j} V_{ij} \\
V_{ij} =& Be^{-\alpha(r_{ij}-z_0)} \\
& + C(1 + D_1\rho_{ij}^2 + D_2\rho_{ij}^4 e^{-\lambda_1\rho_{ij}^2} e^{-\lambda_2(z_{ij}^2-z_0^2)} \\
& - A\left(\frac{z_0}{r_ij}\right)^6 + A\left(\frac{z_0}{r_c}\right)^6 \\
\rho_{ij}^2 =& x_{ij}^2 + y_{ij}^2 \qquad (\mathbf{n_i} \equiv \hat{\mathbf{z}})
\end{aligned}
$$

It is important to have a sufficiently large cutoff to ensure smooth forces. Energies are shifted so that they go continuously to zero at the cutoff assuming that the exponential part of V_{ij} (first term) decays sufficiently fast. This shift is achieved by the last term in the equation for V_{ij} above.

The parameter file (e.g. CC.Lebedeva), is intended for use with metal *units*, with energies in meV. An additional parameter, *S*, is available to facilitate scaling of energies.

This potential must be used in combination with hybrid/overlay. Other interactions can be set to zero using pair_style *none*.

18.246.4 Restrictions

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.246.5 Related commands

pair_coeff, *pair_style none*, *pair_style hybrid/overlay*, *pair_style drip*, *pair_style ilp/graphene/hbd*, *pair_style kolmogorov/crespi/z*, *pair_style kolmogorov/crespi/full*.

Default: none

(Lebedeva et al.) I. V. Lebedeva, A. A. Knizhnik, A. M. Popov, Y. E. Lozovik, B. V. Potapkin, Phys. Rev. B, 84, 245437 (2011)

18.247 pair_style line/lj command

18.247.1 Syntax

```
pair_style line/lj cutoff
```

cutoff = global cutoff for interactions (distance units)

18.247.2 Examples

```
pair_style line/lj 3.0
pair_coeff * * 1.0 1.0 1.0 0.8 1.12
pair_coeff 1 2 1.0 2.0 1.0 1.5 1.12 5.0
pair_coeff 1 2 1.0 0.0 1.0 1.0 2.5
```

18.247.3 Description

Style *line/lj* treats particles which are line segments as a set of small spherical particles that tile the line segment length as explained below. Interactions between two line segments, each with N1 and N2 spherical particles, are calculated as the pairwise sum of N1*N2 Lennard-Jones interactions. Interactions between a line segment with N spherical particles and a point particle are treated as the pairwise sum of N Lennard-Jones interactions. See the *pair_style lj/cut* doc page for the definition of Lennard-Jones interactions.

The set of non-overlapping spherical sub-particles that represent a line segment are generated in the following manner. Their size is a function of the line segment length and the specified sub-particle size for that particle type. If a line segment has a length L and is of type I, then the number of spheres N that represent the segment is calculated as N = L/sizeI, rounded up to an integer value. Thus if L is not evenly divisible by sizeI, N is incremented to include one extra sphere. The centers of the spheres are spaced equally along the line segment. Imagine N+1 equally-space points, which include the 2 end points of the segment. The sphere centers are halfway between each pair of points.

The LJ interaction between 2 spheres on different line segments (or a sphere on a line segment and a point particles) is computed with sub-particle ϵ, σ, and *cutoff* values that are set by the pair_coeff command, as described below. If the distance between the 2 spheres is greater than the sub-particle cutoff, there is no interaction. This means that some pairs of sub-particles on 2 line segments may interact, but others may not.

For purposes of creating the neighbor list for pairs of interacting line segments or lines/point particles, a regular particle-particle cutoff is used, as defined by the *cutoff* setting above in the pair_style command or overridden with an optional argument in the pair_coeff command for a type pair as discussed below. The distance between the centers of 2 line segments, or the center of a line segment and a point particle, must be less than this distance (plus the neighbor skin; see the *neighbor* command), for the pair of particles to be included in the neighbor list.

Note: This means that a too-short value for the *cutoff* setting can exclude a pair of particles from the neighbor list even if pairs of their sub-particle spheres would interact, based on the sub-particle cutoff specified in the pair_coeff command. E.g. sub-particles at the ends of the line segments that are close to each other. Which may not be what you want, since it means the ends of 2 line segments could pass through each other. It is up to you to specify a *cutoff* setting that is consistent with the length of the line segments you are using and the sub-particle cutoff settings.

For style *line/lj*, the following coefficients must be defined for each pair of atom types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- sizeI (distance units)
- sizeJ (distance units)
- ϵ (energy units)
- σ (distance units)
- subcutoff (distance units)
- cutoff (distance units)

The *sizeI* and *sizeJ* coefficients are the sub-particle sizes for line particles of type I and type J. They are used to define the N sub-particles per segment as described above. These coefficients are actually stored on a per-type basis. Thus if there are multiple pair_coeff commands that involve type I, as either the first or second atom type, you should use consistent values for sizeI or sizeJ in all of them. If you do not do this, the last value specified for sizeI will apply to all segments of type I. If typeI or typeJ refers to point particles, the corresponding sizeI or sizeJ is ignored; it can be set to 0.0.

The ϵ, σ, and *subcutoff* coefficients are used to compute an LJ interactions between a pair of sub-particles on 2 line segments (of type I and J), or between a sub particle/point particle pair. As discussed above, the *subcutoff* and *cutoff* params are different. The latter is only used for building the neighbor list when the distance between centers of two line segments or one segment and a point particle is calculated.

The *cutoff* coefficient is optional. If not specified, the global cutoff is used.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, coefficients must be specified. No default mixing rules are used.

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style does not write its information to *binary restart files*.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.247.4 Restrictions

This style is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Defining particles to be line segments so they participate in line/line or line/particle interactions requires the use the *atom_style line* command.

18.247.5 Related commands

pair_coeff, *pair_style tri/lj*

Default: none

18.248 pair_style list command

18.248.1 Syntax

```
pair_style list listfile cutoff keyword
```

- listfile = name of file with list of pairwise interactions
- cutoff = global cutoff (distance units)
- keyword = optional flag *nocheck* or *check* (default is *check*)

18.248.2 Examples

```
pair_style list restraints.txt 200.0
pair_coeff * *

pair_style hybrid/overlay lj/cut 1.1225 list pair_list.txt 300.0
pair_coeff * * lj/cut 1.0 1.0
pair_coeff 3* 3* list
```

18.248.3 Description

Style *list* computes interactions between explicitly listed pairs of atoms with the option to select functional form and parameters for each individual pair. Because the parameters are set in the list file, the pair_coeff command has no parameters (but still needs to be provided). The *check* and *nocheck* keywords enable/disable a test that checks whether all listed bonds were present and computed.

This pair style can be thought of as a hybrid between bonded, non-bonded, and restraint interactions. It will typically be used as an additional interaction within the *hybrid/overlay* pair style. It currently supports three interaction styles: a 12-6 Lennard-Jones, a Morse and a harmonic potential.

The format of the list file is as follows:

- one line per pair of atoms
- empty lines will be ignored
- comment text starts with a '#' character
- line syntax: *ID1 ID2 style coeffs cutoff*

```
ID1 = atom ID of first atom
ID2 = atom ID of second atom
style = style of interaction
coeffs = list of coeffs
cutoff = cutoff for interaction (optional)
```

The cutoff parameter is optional. If not specified, the global cutoff is used.

Here is an example file:

```
# this is a comment

15 259 lj126     1.0 1.0      50.0
15 603 morse    10.0 1.2 2.0  10.0 # and another comment
18 470 harmonic 50.0 1.2       5.0
```

The style *lj126* computes pairwise interactions with the formula

$$E = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \qquad r < r_c$$

and the coefficients:

- ϵ (energy units)
- σ (distance units)

The style *morse* computes pairwise interactions with the formula

$$E = D_0 \left[e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)} \right] \qquad r < r_c$$

and the coefficients:

- D_0 (energy units)
- α (1/distance units)
- r_0 (distance units)

The style *harmonic* computes pairwise interactions with the formula

$$E = K(r - r_0)^2$$

and the coefficients:

- K (energy units)
- r_0 (distance units)

Note that the usual 1/2 factor is included in K.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support mixing since all parameters are explicit for each pair.

The *pair_modify* shift option is supported by this pair style.

The *pair_modify* table and tail options are not relevant for this pair style.

This pair style does not write its information to *binary restart files*, so pair_style and pair_coeff commands need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.248.4 Restrictions

This pair style does not use a neighbor list and instead identifies atoms by their IDs. This has two consequences: 1) The cutoff has to be chosen sufficiently large, so that the second atom of a pair has to be a ghost atom on the same node on which the first atom is local; otherwise the interaction will be skipped. You can use the *check* option to detect, if interactions are missing. 2) Unlike other pair styles in LAMMPS, an atom I will not interact with multiple images of atom J (assuming the images are within the cutoff distance), but only with the nearest image.

This style is part of the USER-MISC package. It is only enabled if LAMMPS is build with that package. See the *Build package* doc page on for more info.

18.248.5 Related commands

pair_coeff, *pair_style hybrid/overlay*, *pair_style lj/cut*, *pair_style morse*, *bond_style harmonic*

Default: none

18.249 pair_style lj/cut command

18.250 pair_style lj/cut/gpu command

18.251 pair_style lj/cut/intel command

18.252 pair_style lj/cut/kk command

18.253 pair_style lj/cut/opt command

18.254 pair_style lj/cut/omp command

18.255 pair_style lj/cut/coul/cut command

18.256 pair_style lj/cut/coul/cut/gpu command

18.257 pair_style lj/cut/coul/cut/kk command

18.258 pair_style lj/cut/coul/cut/omp command

18.259 pair_style lj/cut/coul/debye command

18.260 pair_style lj/cut/coul/debye/gpu command

18.261 pair_style lj/cut/coul/debye/kk command

18.262 pair_style lj/cut/coul/debye/omp command

18.263 pair_style lj/cut/coul/dsf command

18.264 pair_style lj/cut/coul/dsf/gpu command

18.265 pair_style lj/cut/coul/dsf/kk command

18.266 pair_style lj/cut/coul/dsf/omp command

18.267 pair_style lj/cut/coul/long command

18.268 pair_style lj/cut/coul/long/gpu command

18.269 pair_style lj/cut/coul/long/kk command

18.270 pair_style lj/cut/coul/long/intel command

```
pair_style style args
```

- style = *lj/cut* or *lj/cut/coul/cut* or *lj/cut/coul/debye* or *lj/cut/coul/dsf* or *lj/cut/coul/long* *lj/cut/coul/msm* or *lj/cut/tip4p/long*
- args = list of arguments for a particular style

```
lj/cut args = cutoff
  cutoff = global cutoff for Lennard Jones interactions (distance units)
lj/cut/coul/cut args = cutoff (cutoff2)
  cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
lj/cut/coul/debye args = kappa cutoff (cutoff2)
  kappa = inverse of the Debye length (inverse distance units)
  cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
lj/cut/coul/dsf args = alpha cutoff (cutoff2)
  alpha = damping parameter (inverse distance units)
  cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
  cutoff2 = global cutoff for Coulombic (distance units)
lj/cut/coul/long args = cutoff (cutoff2)
  cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
lj/cut/coul/msm args = cutoff (cutoff2)
  cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
lj/cut/coul/wolf args = alpha cutoff (cutoff2)
  alpha = damping parameter (inverse distance units)
  cutoff = global cutoff for LJ (and Coulombic if only 2 arg) (distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
lj/cut/tip4p/cut args = otype htype btype atype qdist cutoff (cutoff2)
  otype,htype = atom types for TIP4P O and H
  btype,atype = bond and angle types for TIP4P waters
  qdist = distance from O atom to massless charge (distance units)
  cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
lj/cut/tip4p/long args = otype htype btype atype qdist cutoff (cutoff2)
  otype,htype = atom types for TIP4P O and H
  btype,atype = bond and angle types for TIP4P waters
  qdist = distance from O atom to massless charge (distance units)
  cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
```

18.283.2 Examples

```
pair_style lj/cut 2.5
pair_coeff * * 1 1
pair_coeff 1 1 1 1.1 2.8

pair_style lj/cut/coul/cut 10.0
pair_style lj/cut/coul/cut 10.0 8.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0
```

(continues on next page)

(continued from previous page)

```
pair_coeff 1 1 100.0 3.5 9.0 9.0

pair_style lj/cut/coul/debye 1.5 3.0
pair_style lj/cut/coul/debye 1.5 2.5 5.0
pair_coeff * * 1.0 1.0
pair_coeff 1 1 1.0 1.5 2.5
pair_coeff 1 1 1.0 1.5 2.5 5.0

pair_style lj/cut/coul/dsf 0.05 2.5 10.0
pair_coeff * * 1.0 1.0
pair_coeff 1 1 1.0 1.0 2.5

pair_style lj/cut/coul/long 10.0
pair_style lj/cut/coul/long 10.0 8.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0

pair_style lj/cut/coul/msm 10.0
pair_style lj/cut/coul/msm 10.0 8.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0

pair_style lj/cut/tip4p/cut 1 2 7 8 0.15 12.0
pair_style lj/cut/tip4p/cut 1 2 7 8 0.15 12.0 10.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0

pair_style lj/cut/coul/wolf 0.2 5. 10.0
pair_coeff * * 1.0 1.0
pair_coeff 1 1 1.0 1.0 2.5

pair_style lj/cut/tip4p/long 1 2 7 8 0.15 12.0
pair_style lj/cut/tip4p/long 1 2 7 8 0.15 12.0 10.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0
```

18.283.3 Description

The *lj/cut* styles compute the standard 12/6 Lennard-Jones potential, given by

$$E = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \qquad r < r_c$$

Rc is the cutoff.

Style *lj/cut/coul/cut* adds a Coulombic pairwise interaction given by

$$E = \frac{C q_i q_j}{\epsilon r} \qquad r < r_c$$

where C is an energy-conversion constant, q_i and q_j are the charges on the 2 atoms, and ϵ is the dielectric constant which can be set by the *dielectric* command. If one cutoff is specified in the pair_style command, it is used for both the LJ and Coulombic terms. If two cutoffs are specified, they are used as cutoffs for the LJ and Coulombic terms respectively.

Style *lj/cut/coul/debye* adds an additional exp() damping factor to the Coulombic term, given by

$$E = \frac{C q_i q_j}{\epsilon r} \exp(-\kappa r) \qquad r < r_c$$

where κ is the inverse of the Debye length. This potential is another way to mimic the screening effect of a polar solvent.

Style *lj/cut/coul/dsf* computes the Coulombic term via the damped shifted force model described in *Fennell*, given by:

$$E = q_i q_j \left[\frac{\mathrm{erfc}(\alpha r)}{r} - \frac{\mathrm{erfc}(\alpha r_c)}{r_c} + \left(\frac{\mathrm{erfc}(\alpha r_c)}{r_c^2} + \frac{2\alpha}{\sqrt{\pi}} \frac{\exp(-\alpha^2 r_c^2)}{r_c} \right) (r - r_c) \right] \qquad r < r_c$$

where α is the damping parameter and erfc() is the complementary error-function. This potential is essentially a short-range, spherically-truncated, charge-neutralized, shifted, pairwise *1/r* summation. The potential is based on Wolf summation, proposed as an alternative to Ewald summation for condensed phase systems where charge screening causes electrostatic interactions to become effectively short-ranged. In order for the electrostatic sum to be absolutely convergent, charge neutralization within the cutoff radius is enforced by shifting the potential through placement of image charges on the cutoff sphere. Convergence can often be improved by setting α to a small non-zero value.

Styles *lj/cut/coul/long* and *lj/cut/coul/msm* compute the same Coulombic interactions as style *lj/cut/coul/cut* except that an additional damping factor is applied to the Coulombic term so it can be used in conjunction with the *kspace_style* command and its *ewald* or *pppm* option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

Style *coul/wolf* adds a Coulombic pairwise interaction via the Wolf summation method, described in *Wolf*, given by:

$$E_i = \frac{1}{2} \sum_{j \neq i} \frac{q_i q_j \mathrm{erfc}(\alpha r_{ij})}{r_{ij}} + \frac{1}{2} \sum_{j \neq i} \frac{q_i q_j \mathrm{erf}(\alpha r_{ij})}{r_{ij}} \qquad r < r_c$$

where α is the damping parameter, and erfc() is the complementary error-function terms. This potential is essentially a short-range, spherically-truncated, charge-neutralized, shifted, pairwise *1/r* summation. With a manipulation of adding and subtracting a self term (for i = j) to the first and second term on the right-hand-side, respectively, and a small enough α damping parameter, the second term shrinks and the potential becomes a rapidly-converging real-space summation. With a long enough cutoff and small enough α parameter, the energy and forces calculated by the Wolf summation method approach those of the Ewald sum. So it is a means of getting effective long-range interactions with a short-range potential.

Styles *lj/cut/tip4p/cut* and *lj/cut/tip4p/long* implement the TIP4P water model of *(Jorgensen)*, which introduces a massless site located a short distance away from the oxygen atom along the bisector of the HOH angle. The atomic types of the oxygen and hydrogen atoms, the bond and angle types for OH and HOH interactions, and the distance to the massless charge site are specified as pair_style arguments. Style *lj/cut/tip4p/cut* uses a cutoff for Coulomb interactions; style *lj/cut/tip4p/long* is for use with a long-range Coulombic solver (Ewald or PPPM).

Note: For each TIP4P water molecule in your system, the atom IDs for the O and 2 H atoms must be consecutive, with the O atom first. This is to enable LAMMPS to "find" the 2 H atoms associated with each O atom. For example, if the atom ID of an O atom in a TIP4P water molecule is 500, then its 2 H atoms must have IDs 501 and 502.

See the *Howto tip4p* doc page for more information on how to use the TIP4P pair styles and lists of parameters to set. Note that the neighbor list cutoff for Coulomb interactions is effectively extended by a distance 2*qdist when using the TIP4P pair style, to account for the offset distance of the fictitious charges on O atoms in water molecules. Thus it is typically best in an efficiency sense to use a LJ cutoff >= Coulombic cutoff + 2*qdist, to shrink the size of the neighbor list. This leads to slightly larger cost for the long-range calculation, so you can test the trade-off for your model.

For all of the *lj/cut* pair styles, the following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- ϵ (energy units)
- σ (distance units)

- cutoff1 (distance units)
- cutoff2 (distance units)

Note that σ is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum at $2^{\frac{1}{6}}\sigma$.

The latter 2 coefficients are optional. If not specified, the global LJ and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both LJ and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the LJ and Coulombic cutoffs for this type pair. You cannot specify 2 cutoffs for style *lj/cut*, since it has no Coulombic terms.

For *lj/cut/coul/long* and *lj/cut/coul/msm* and *lj/cut/tip4p/cut* and *lj/cut/tip4p/long* only the LJ cutoff can be specified since a Coulombic cutoff cannot be specified for an individual I,J type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

A version of these styles with a soft core, *lj/cut/soft*, suitable for use in free energy calculations, is part of the USER-FEP package and is documented with the *pair_style */soft* styles. The version with soft core is only available if LAMMPS was built with that package. See the *Build package* doc page for more info.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/cut pair styles can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

All of the *lj/cut* pair styles support the *pair_modify* shift option for the energy of the Lennard-Jones portion of the pair interaction.

The *lj/cut/coul/long* and *lj/cut/tip4p/long* pair styles support the *pair_modify* table option since they can tabulate the short-range portion of the long-range Coulombic interaction.

All of the *lj/cut* pair styles support the *pair_modify* tail option for adding a long-range tail correction to the energy and pressure for the Lennard-Jones portion of the pair interaction.

All of the *lj/cut* pair styles write their information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

The *lj/cut* and *lj/cut/coul/long* pair styles support the use of the *inner*, *middle*, and *outer* keywords of the *run_style respa* command, meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. The other styles only support the *pair* keyword of run_style respa. See the *run_style* command for details.

18.283.4 Restrictions

The *lj/cut/coul/long* and *lj/cut/tip4p/long* styles are part of the KSPACE package. The *lj/cut/tip4p/cut* style is part of the MOLECULE package. These styles are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

18.283.5 Related commands

pair_coeff

Default: none

(Jorgensen) Jorgensen, Chandrasekhar, Madura, Impey, Klein, J Chem Phys, 79, 926 (1983).

(Fennell) C. J. Fennell, J. D. Gezelter, J Chem Phys, 124, 234104 (2006).

18.284 pair_style lj96/cut command

18.285 pair_style lj96/cut/gpu command

18.286 pair_style lj96/cut/omp command

18.286.1 Syntax

```
pair_style lj96/cut cutoff
```

- cutoff = global cutoff for lj96/cut interactions (distance units)

18.286.2 Examples

```
pair_style lj96/cut 2.5
pair_coeff * * 1.0 1.0 4.0
pair_coeff 1 1 1.0 1.0
```

18.286.3 Description

The *lj96/cut* style compute a 9/6 Lennard-Jones potential, instead of the standard 12/6 potential, given by

$$E = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^9 - \left(\frac{\sigma}{r}\right)^6 \right] \qquad r < r_c$$

r_c is the cutoff.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- ϵ (energy units)

- σ (distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global LJ cutoff specified in the pair_style command is used.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/cut pair styles can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style supports the *pair_modify* shift option for the energy of the pair interaction.

The *pair_modify* table option is not relevant for this pair style.

This pair style supports the *pair_modify* tail option for adding a long-range tail correction to the energy and pressure of the pair interaction.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style supports the use of the *inner*, *middle*, and *outer* keywords of the *run_style respa* command, meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. See the *run_style* command for details.

18.286.4 Restrictions

none

18.286.5 Related commands

pair_coeff

Default: none

18.287 pair_style lj/cubic command

18.288 pair_style lj/cubic/gpu command

18.289 pair_style lj/cubic/omp command

18.289.1 Syntax

```
pair_style lj/cubic
```

18.289.2 Examples

```
pair_style lj/cubic
pair_coeff * * 1.0 0.8908987
```

18.289.3 Description

The *lj/cubic* style computes a truncated LJ interaction potential whose energy and force are continuous everywhere. Inside the inflection point the interaction is identical to the standard 12/6 *Lennard-Jones* potential. The LJ function outside the inflection point is replaced with a cubic function of distance. The energy, force, and second derivative are continuous at the inflection point. The cubic coefficient A3 is chosen so that both energy and force go to zero at the cutoff distance. Outside the cutoff distance the energy and force are zero.

$$
\begin{aligned}
E &= u_{LJ}(r) \qquad r \le r_s \\
&= u_{LJ}(r_s) + (r - r_s)u'_{LJ}(r_s) - \frac{1}{6}A_3(r - r_s)^3 \qquad r_s < r \le r_c \\
&= 0 \qquad r > r_c
\end{aligned}
$$

The location of the inflection point r_s is defined by the LJ diameter, $r_s/\sigma = (26/7)^{1/6}$. The cutoff distance is defined by $r_c/r_s = 67/48$ or $r_c/\sigma = 1.737...$ The analytic expression for the the cubic coefficient $A_3 r_{min}^3/\epsilon = 27.93...$ is given in the paper by Holian and Ravelo *(Holian)*.

This potential is commonly used to study the shock mechanics of FCC solids, as in Ravelo et al. *(Ravelo)*.

The following coefficients must be defined for each pair of atom types via the *pair_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- ϵ (energy units)
- σ (distance units)

Note that σ is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum, which is located at $r_{min} = 2^{\frac{1}{6}}\sigma$. In the above example, $\sigma = 0.8908987$, so $r_{min} = 1.0$.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/cut pair styles can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

The lj/cubic pair style does not support the *pair_modify* shift option, since pair interaction is already smoothed to 0.0 at the cutoff.

The *pair_modify* table option is not relevant for this pair style.

The lj/cubic pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure, since there are no corrections for a potential that goes to 0.0 at the cutoff.

The lj/cubic pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

The lj/cubic pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.289.4 Restrictions

none

18.289.5 Related commands

pair_coeff

Default: none

(Holian) Holian and Ravelo, Phys Rev B, 51, 11275 (1995).

(Ravelo) Ravelo, Holian, Germann and Lomdahl, Phys Rev B, 70, 014103 (2004).

18.290 pair_style lj/expand command

18.291 pair_style lj/expand/gpu command

18.292 pair_style lj/expand/kk command

18.293 pair_style lj/expand/omp command

18.294 pair_style lj/expand/coul/long command

18.295 pair_style lj/expand/coul/long/gpu command

18.295.1 Syntax

```
pair_style lj/expand cutoff
```

- cutoff = global cutoff for lj/expand interactions (distance units)

18.295.2 Examples

```
pair_style lj/expand 2.5
pair_coeff * * 1.0 1.0 0.5
pair_coeff 1 1 1.0 1.0 -0.2 2.0

pair_style lj/expand/coul/long 2.5
pair_style lj/expand/coul/long 2.5 4.0
pair_coeff * * 1.0 1.0 0.5
pair_coeff 1 1 1.0 1.0 -0.2 3.0
```

18.295.3 Description

Style *lj/expand* computes a LJ interaction with a distance shifted by delta which can be useful when particles are of different sizes, since it is different that using different sigma values in a standard LJ formula:

$$E = 4\epsilon \left[\left(\frac{\sigma}{r - \Delta} \right)^{12} - \left(\frac{\sigma}{r - \Delta} \right)^{6} \right] \qquad r < r_c + \Delta$$

r_c is the cutoff which does not include the Δ distance. I.e. the actual force cutoff is the sum of $r_c + \Delta$.

For all of the *lj/expand* pair styles, the following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- ϵ (energy units)
- σ (distance units)
- Δ (distance units)

- cutoff (distance units)

The Δ values can be positive or negative. The last coefficient is optional. If not specified, the global LJ cutoff is used.

For *lj/expand/coul/long* only the LJ cutoff can be specified since a Coulombic cutoff cannot be specified for an individual I,J type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon, sigma, and shift coefficients and cutoff distance for this pair style can be mixed. Shift is always mixed via an *arithmetic* rule. The other coefficients are mixed according to the pair_modify mix value. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style supports the *pair_modify* shift option for the energy of the pair interaction.

The *pair_modify* table option is not relevant for this pair style.

This pair style supports the *pair_modify* tail option for adding a long-range tail correction to the energy and pressure of the pair interaction.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.295.4 Restrictions

none

18.295.5 Related commands

pair_coeff

Default: none

18.296 pair_style lj/long/coul/long command

18.297 pair_style lj/long/coul/long/intel command

18.298 pair_style lj/long/coul/long/omp command

18.299 pair_style lj/long/coul/long/opt command

18.300 pair_style lj/long/tip4p/long command

18.301 pair_style lj/long/tip4p/long/omp command

18.301.1 Syntax

```
pair_style style args
```

- style = *lj/long/coul/long* or *lj/long/tip4p/long*
- args = list of arguments for a particular style

```
lj/long/coul/long args = flag_lj flag_coul cutoff (cutoff2)
  flag_lj = long or cut or off
    long = use Kspace long-range summation for dispersion 1/r^6 term
    cut = use a cutoff on dispersion 1/r^6 term
    off = omit disperion 1/r^6 term entirely
  flag_coul = long or off
    long = use Kspace long-range summation for Coulombic 1/r term
    off = omit Coulombic term
  cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
lj/long/tip4p/long args = flag_lj flag_coul otype htype btype atype qdist␣
↪cutoff (cutoff2)
  flag_lj = long or cut
    long = use Kspace long-range summation for dispersion 1/r^6 term
    cut = use a cutoff
  flag_coul = long or off
    long = use Kspace long-range summation for Coulombic 1/r term
    off = omit Coulombic term
  otype,htype = atom types for TIP4P O and H
  btype,atype = bond and angle types for TIP4P waters
  qdist = distance from O atom to massless charge (distance units)
  cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
```

18.301.2 Examples

```
pair_style lj/long/coul/long cut off 2.5
pair_style lj/long/coul/long cut long 2.5 4.0
pair_style lj/long/coul/long long long 2.5 4.0
pair_coeff * * 1 1
pair_coeff 1 1 1 3 4

pair_style lj/long/tip4p/long long long 1 2 7 8 0.15 12.0
pair_style lj/long/tip4p/long long long 1 2 7 8 0.15 12.0 10.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0
```

18.301.3 Description

Style *lj/long/coul/long* computes the standard 12/6 Lennard-Jones potential:

$$E = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \qquad r < r_c$$

with ϵ and σ being the usual Lennard-Jones potential parameters, plus the Coulomb potential, given by:

$$E = \frac{C q_i q_j}{\epsilon r} \qquad r < r_c$$

where C is an energy-conversion constant, q_i and q_j are the charges on the 2 atoms, ϵ is the dielectric constant which can be set by the *dielectric* command, and r_c is the cutoff. If one cutoff is specified in the pair_style command, it is used for both the LJ and Coulombic terms. If two cutoffs are specified, they are used as cutoffs for the LJ and Coulombic terms respectively.

The purpose of this pair style is to capture long-range interactions resulting from both attractive 1/r^6 Lennard-Jones and Coulombic 1/r interactions. This is done by use of the *flag_lj* and *flag_coul* settings. The *In 't Veld* paper has more details on when it is appropriate to include long-range 1/r^6 interactions, using this potential.

Style *lj/long/tip4p/long* implements the TIP4P water model of *(Jorgensen)*, which introduces a massless site located a short distance away from the oxygen atom along the bisector of the HOH angle. The atomic types of the oxygen and hydrogen atoms, the bond and angle types for OH and HOH interactions, and the distance to the massless charge site are specified as pair_style arguments.

Note: For each TIP4P water molecule in your system, the atom IDs for the O and 2 H atoms must be consecutive, with the O atom first. This is to enable LAMMPS to "find" the 2 H atoms associated with each O atom. For example, if the atom ID of an O atom in a TIP4P water molecule is 500, then its 2 H atoms must have IDs 501 and 502.

See the *Howto tip4p* doc page for more information on how to use the TIP4P pair style. Note that the neighbor list cutoff for Coulomb interactions is effectively extended by a distance 2*qdist when using the TIP4P pair style, to account for the offset distance of the fictitious charges on O atoms in water molecules. Thus it is typically best in an efficiency sense to use a LJ cutoff >= Coulombic cutoff + 2*qdist, to shrink the size of the neighbor list. This leads to slightly larger cost for the long-range calculation, so you can test the trade-off for your model.

If *flag_lj* is set to *long*, no cutoff is used on the LJ 1/r^6 dispersion term. The long-range portion can be calculated by using the *kspace_style ewald/disp or pppm/disp* commands. The specified LJ cutoff then determines which portion of the LJ interactions are computed directly by the pair potential versus which part is computed in reciprocal space via the Kspace style. If *flag_lj* is set to *cut*, the LJ interactions are simply cutoff, as with *pair_style lj/cut*.

If *flag_coul* is set to *long*, no cutoff is used on the Coulombic interactions. The long-range portion can calculated by using any of several *kspace_style* command options such as *pppm* or *ewald*. Note that if *flag_lj* is also set to long, then

the *ewald/disp* or *pppm/disp* Kspace style needs to be used to perform the long-range calculations for both the LJ and Coulombic interactions. If *flag_coul* is set to *off*, Coulombic interactions are not computed.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- ϵ (energy units)
- σ (distance units)
- cutoff1 (distance units)
- cutoff2 (distance units)

Note that sigma is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum at 2^(1/6) sigma.

The latter 2 coefficients are optional. If not specified, the global LJ and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both LJ and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the LJ and Coulombic cutoffs for this type pair.

Note that if you are using *flag_lj* set to *long*, you cannot specify a LJ cutoff for an atom type pair, since only one global LJ cutoff is allowed. Similarly, if you are using *flag_coul* set to *long*, you cannot specify a Coulombic cutoff for an atom type pair, since only one global Coulombic cutoff is allowed.

For *lj/long/tip4p/long* only the LJ cutoff can be specified since a Coulombic cutoff cannot be specified for an individual I,J type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

A version of these styles with a soft core, *lj/cut/soft*, suitable for use in free energy calculations, is part of the USER-FEP package and is documented with the *pair_style */soft* styles. The version with soft core is only available if LAMMPS was built with that package. See the *Build package* doc page for more info.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/long pair styles can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

These pair styles support the *pair_modify* shift option for the energy of the Lennard-Jones portion of the pair interaction, assuming *flag_lj* is *cut*.

These pair styles support the *pair_modify* table and table/disp options since they can tabulate the short-range portion of the long-range Coulombic and dispersion interactions.

Thes pair styles do not support the *pair_modify* tail option for adding a long-range tail correction to the Lennard-Jones portion of the energy and pressure.

These pair styles write their information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

The pair lj/long/coul/long styles support the use of the *inner*, *middle*, and *outer* keywords of the *run_style respa* command, meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. See the *run_style* command for details.

18.301.4 Restrictions

These styles are part of the KSPACE package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.301.5 Related commands

pair_coeff

Default: none

(In 't Veld) In 't Veld, Ismail, Grest, J Chem Phys (accepted) (2007).

(Jorgensen) Jorgensen, Chandrasekhar, Madura, Impey, Klein, J Chem Phys, 79, 926 (1983).

18.302 pair_style lj/smooth command

18.303 pair_style lj/smooth/omp command

18.303.1 Syntax

```
pair_style lj/smooth Rin Rc
```

- Rin = inner cutoff beyond which force smoothing will be applied (distance units)
- Rc = outer cutoff for lj/smooth interactions (distance units)

18.303.2 Examples

```
pair_style lj/smooth 8.0 10.0
pair_coeff * * 10.0 1.5
pair_coeff 1 1 20.0 1.3 7.0 9.0
```

18.303.3 Description

Style *lj/smooth* computes a LJ interaction with a force smoothing applied between the inner and outer cutoff.

$$E = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \qquad r < r_{in}$$
$$F = C_1 + C_2(r - r_{in}) + C_3(r - r_{in})^2 + C_4(r - r_{in})^3 \qquad r_{in} < r < r_c$$

The polynomial coefficients C1, C2, C3, C4 are computed by LAMMPS to cause the force to vary smoothly from the inner cutoff r_{in} to the outer cutoff r_c.

At the inner cutoff the force and its 1st derivative will match the non-smoothed LJ formula. At the outer cutoff the force and its 1st derivative will be 0.0. The inner cutoff cannot be 0.0.

Note: this force smoothing causes the energy to be discontinuous both in its values and 1st derivative. This can lead to poor energy conservation and may require the use of a thermostat. Plot the energy and force resulting from this formula via the *pair_write* command to see the effect.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- ϵ (energy units)
- σ (distance units)
- r_{in} (distance units)
- r_c (distance units)

The last 2 coefficients are optional inner and outer cutoffs. If not specified, the global values for r_{in} and r_c are used.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon, sigma, Rin coefficients and the cutoff distance for this pair style can be mixed. Rin is a cutoff value and is mixed like the cutoff. The other coefficients are mixed according to the pair_modify mix option. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style supports the *pair_modify* shift option for the energy of the pair interaction.

The *pair_modify* table option is not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure, since the energy of the pair interaction is smoothed to 0.0 at the cutoff.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.303.4 Restrictions

none

18.303.5 Related commands

pair_coeff, *pair lj/smooth/linear*

Default: none

18.304 pair_style lj/smooth/linear command

18.305 pair_style lj/smooth/linear/omp command

18.305.1 Syntax

```
pair_style lj/smooth/linear cutoff
```

- cutoff = global cutoff for Lennard-Jones interactions (distance units)

18.305.2 Examples

```
pair_style lj/smooth/linear 2.5
pair_coeff * * 1.0 1.0
pair_coeff 1 1 0.3 3.0 9.0
```

18.305.3 Description

Style *lj/smooth/linear* computes a truncated and force-shifted LJ interaction (aka Shifted Force Lennard-Jones) that combines the standard 12/6 Lennard-Jones function and subtracts a linear term based on the cutoff distance, so that both, the potential and the force, go continuously to zero at the cutoff Rc *(Toxvaerd)*:

$$\phi(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

$$E(r) = \phi(r) - \phi(R_c) - (r - R_c) \left.\frac{d\phi}{dr}\right|_{r=R_c} \qquad r < R_c$$

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- ϵ (energy units)
- σ (distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global LJ cutoff specified in the pair_style command is used.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance can be mixed. The default mix value is geometric. See the "pair_modify" command for details.

This pair style does not support the *pair_modify* shift option for the energy of the pair interaction, since it goes to 0.0 at the cutoff by construction.

The *pair_modify* table option is not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure, since the energy of the pair interaction is smoothed to 0.0 at the cutoff.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.305.4 Restrictions

none

18.305.5 Related commands

pair_coeff, *pair lj/smooth*

Default: none

(Toxvaerd) Toxvaerd, Dyre, J Chem Phys, 134, 081102 (2011).

18.306 pair_style lj/switch3/coulgauss/long command

18.306.1 Syntax

```
pair_style style args
```

- style = *lj/switch3/coulgauss/long*
- args = list of arguments for a particular style

```
lj/switch3/coulgauss/long args = cutoff (cutoff2) width
  cutoff  = global cutoff for LJ (and Coulombic if only 1 arg) (distance␣
↪units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
  width  = width parameter of the smoothing function (distance units)
```

18.306.2 Examples

```
pair_style lj/switch3/coulgauss/long    12.0 3.0
pair_coeff 1  0.2 2.5 1.2

pair_style lj/switch3/coulgauss/long   12.0 10.0 3.0
pair_coeff 1  0.2 2.5 1.2
```

18.306.3 Description

The *lj/switch3/coulgauss* style evaluates the LJ vdW potential

$$E = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

, which goes smoothly to zero at the cutoff r_c as defined by the switching function

$$S_3(r) = \begin{cases} 1 & \text{if} \quad r < r_\mathrm{c} - w \\ 3x^2 - 2x^3 & \text{if} \quad r < r_\mathrm{c} \quad \text{with} \quad x = \frac{r_\mathrm{c} - r}{w} \\ 0 & \text{if} \quad r >= r_\mathrm{c} \end{cases}$$

where w is the width defined in the arguments. This potential is combined with Coulomb interaction between Gaussian charge densities:

$$E = \frac{q_i q_j \mathrm{erf}\left(r/\sqrt{\gamma_1^2 + \gamma_2^2}\right)}{\epsilon r_{ij}}$$

where q_i and q_j are the charges on the 2 atoms, ϵ is the dielectric constant which can be set by the *dielectric* command, γ_i and γ_j are the widths of the Gaussian charge distribution and erf() is the error-function. This style has to be used in conjunction with the *kspace_style* command

If one cutoff is specified it is used for both the vdW and Coulomb terms. If two cutoffs are specified, the first is used as the cutoff for the vdW terms, and the second is the cutoff for the Coulombic term.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- ϵ (energy)

- σ (distance)
- γ (distance)

Mixing, shift, table, tail correction, restart, rRESPA info:

Shifting the potential energy is not necessary because the switching function ensures that the potential is zero at the cut-off.

18.306.4 Restrictions

These styles are part of the USER-YAFF package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.306.5 Related commands

pair_coeff

Default: none

18.307 pair_style local/density command

18.307.1 Syntax

```
pair_style style arg
```

- style = *local/density*
- arg = name of file containing tabulated values of local density and the potential

18.307.2 Examples

```
pair_style local/density benzene_water.localdensity.table

pair_style hybrid/overlay table spline 500 local/density
pair_coeff * * local/density  benzene_water.localdensity.table
```

18.307.3 Description

The local density (LD) potential is a mean-field manybody potential, and, in some sense,a generalization of embedded atom models (EAM). The name "local density potential" arises from the fact that it assigns an energy to an atom depending on the number of neighboring atoms of given type around it within a predefined spherical volume (i.e., within a cutoff). The bottom-up coarse-graining (CG) literature suggests that such potentials can be widely useful in capturing effective multibody forces in a computationally efficient manner so as to improve the quality of CG models of implicit solvation:ref:*(Sanyal1)* <*Sanyal1*> and phase-segregation in liquid mixtures:ref:*(Sanyal2)* <*Sanyal2*>, and provide guidelines to determine the extent of manybody correlations present in a CG model.:ref:*(Rosenberger)* <*Rosenberger*> The LD potential in LAMMPS is primarily intended to be used as a corrective potential over traditional pair potentials in bottom-up CG models, i.e., as a hybrid pair style with other explicit pair interaction terms (e.g.,

table spline, Lennard Jones, etc.). Because the LD potential is not a pair potential per se, it is implemented simply as a single auxiliary file with all specifications that will be read upon initialization.

Note: Thus when used as the only interaction in the system, there is no corresponding pair_coeff command and when used with other pair styles using the hybrid/overlay option, the corresponding pair_coeff command must be supplied * * as placeholders for the atom types.

System with a single CG atom type:

A system of a single atom type (e.g., LJ argon) with a single local density (LD) potential would have an energy given by:

$$U_{LD} = \sum_i F(\rho_i)$$

where ρ_i is the LD at atom *i* and $F(\rho)$ is similar in spirit to the embedding function used in EAM potentials. The LD at atom *i* is given by the sum

$$\rho_i = \sum_{j \neq i} \varphi(r_{ij})$$

where φ is an indicator function that is one at r=0 and zero beyond a cutoff distance R2. The choice of the functional form of φ is somewhat arbitrary, but the following piecewise cubic function has proven sufficiently general: *(Sanyal1)*, *(Sanyal2)* *(Rosenberger)*

$$\varphi(r) = \begin{cases} 1 & r \leq R_1 \\ c_0 + c_2 r^2 + c_4 r^4 + c_6 r^6 & r \in (R_1, R_2) \\ 0 & r \geq R_2 \end{cases}$$

The constants *c* are chosen so that the indicator function smoothly interpolates between 1 and 0 between the distances R1 and R2, which are called the inner and outer cutoffs, respectively. Thus phi satisfies phi(R1) = 1, phi(R2) = dphi/dr @ (r=R1) = dphi/dr @ (r=R2) = 0. The embedding function F(rho) may or may not have a closed-form expression. To maintain generality, it is practically represented with a spline-interpolated table over a predetermined range of rho. Outside of that range it simply adopts zero values at the endpoints.

It can be shown that the total force between two atoms due to the LD potential takes the form of a pair force, which motivates its designation as a LAMMPS pair style. Please see *(Sanyal1)* for details of the derivation.

Systems with arbitrary numbers of atom types:

The potential is easily generalized to systems involving multiple atom types:

$$U_{LD} = \sum_i a_\alpha F(\rho_i)$$

with the LD expressed as

$$\rho_i = \sum_{j \neq i} b_\beta \varphi(r_{ij})$$

where α gives the type of atom *i*, β the type of atom *j*, and the coefficients *a* and *b* filter for atom types as specified by the user. *a* is called the central atom filter as it determines to which atoms the potential applies; $a_\alpha = 1$ if the LD potential applies to atom type α else zero. On the other hand, *b* is called the neighbor atom filter because it specifies which atom types to use in the calculation of the LD; $b_\beta = 1$ if atom type β contributes to the LD and zero otherwise.

Note: Note that the potentials need not be symmetric with respect to atom types, which is the reason for two distinct sets of coefficients a and b. An atom type may contribute to the LD but not the potential, or to the potential but not the LD. Such decisions are made by the user and should (ideally) be motivated on physical grounds for the problem at hand.

General form for implementation in LAMMPS:

Of course, a system with many atom types may have many different possible LD potentials, each with their own atom type filters, cutoffs, and embedding functions. The most general form of this potential as implemented in the pair_style local/density is:

$$U_{LD} = \sum_k U_{LD}^{(k)} = \sum_i \left[\sum_k a_\alpha^{(k)} F^{(k)} \left(\rho_i^{(k)} \right) \right]$$

where, k is an index that spans the (arbitrary) number of applied LD potentials N_LD. Each LD is calculated as before with:

$$\rho_i^{(k)} = \sum_j b_\beta^{(k)} \varphi^{(k)}(r_{ij})$$

The superscript on the indicator function phi simply indicates that it is associated with specific values of the cutoff distances R1(k) and R2(k). In summary, there may be N_LD distinct LD potentials. With each potential type (k), one must specify:

- the inner and outer cutoffs as R1 and R2
- the central type filter a(k), where k = 1,2,. . . N_LD
- the neighbor type filter b(k), where k = 1,2,. . . N_LD
- the LD potential function F(k)(rho), typically as a table that is later spline-interpolated

Tabulated input file format:

```
Line 1:             comment or blank (ignored)
Line 2:             comment or blank (ignored)
Line 3:             N_LD N_rho (# of LD potentials and # of tabulated values, single␣
↪space separated)
Line 4:             blank (ignored)
Line 5:             R1(k) R2(k) (lower and upper cutoffs, single space separated)
Line 6:             central-types (central atom types, single space separated)
Line 7:             neighbor-types (neighbor atom types single space separated)
Line 8:             rho_min rho_max drho (min, max and diff. in tabulated rho values,␣
↪single space separated)
Line 9:             F(k)(rho_min + 0.drho)
Line 10:            F(k)(rho_min + 1.drho)
Line 11:            F(k)(rho_min + 2.drho)
...
Line 9+N_rho:       F(k)(rho_min + N_rho . drho)
Line 10+N_rho:      blank (ignored)

Block 2

Block 3

Block N_LD
```

Lines 5 to 9+N_rho constitute the first block. Thus the input file is separated (by blank lines) into N_LD blocks each representing a separate LD potential and each specifying its own upper and lower cutoffs, central and neighbor atoms, and potential. In general, blank lines anywhere are ignored.

Mixing, shift, table, tail correction, restart, info: This pair style does not support automatic mixing. For atom type pairs α, β and α != β, even if LD potentials of type (α, α) and (β, β) are provided, you will need to explicitly provide LD potential types (α, β) and (β, α) if need be (Here, the notation (α, β) means that α is the central atom to which the LD potential is applied and β is the neighbor atom which contributes to the LD potential on α).

This pair style does not support the *pair_modify* shift, table, and tail options.

The local/density pair style does not write its information to *binary restart files*, since it is stored in tabulated potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

18.307.4 Restrictions

The local/density pair style is a part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.307.5 Related commands

pair_coeff

Default: none

(Sanyal1) Sanyal and Shell, Journal of Chemical Physics, 2016, 145 (3), 034109.

(Sanyal2) Sanyal and Shell, Journal of Physical Chemistry B, 122 (21), 5678-5693.

(Rosenberger) Rosenberger, Sanyal, Shell and van der Vegt, Journal of Chemical Physics, 2019, 151 (4), 044111.

18.308 pair_style lubricate command

18.309 pair_style lubricate/omp command

18.310 pair_style lubricate/poly command

18.311 pair_style lubricate/poly/omp command

18.311.1 Syntax

```
pair_style style mu flaglog flagfld cutinner cutoff flagHI flagVF
```

- style = *lubricate* or *lubricate/poly*
- mu = dynamic viscosity (dynamic viscosity units)

- flaglog = 0/1 to exclude/include log terms in the lubrication approximation
- flagfld = 0/1 to exclude/include Fast Lubrication Dynamics (FLD) effects
- cutinner = inner cutoff distance (distance units)
- cutoff = outer cutoff for interactions (distance units)
- flagHI (optional) = 0/1 to exclude/include 1/r hydrodynamic interactions
- flagVF (optional) = 0/1 to exclude/include volume fraction corrections in the long-range isotropic terms

Examples: (all assume radius = 1)

```
pair_style lubricate 1.5 1 1 2.01 2.5
pair_coeff 1 1 2.05 2.8
pair_coeff * *

pair_style lubricate 1.5 1 1 2.01 2.5
pair_coeff * *
variable mu equal ramp(1,2)
fix 1 all adapt 1 pair lubricate mu * * v_mu
```

18.311.2 Description

Styles *lubricate* and *lubricate/poly* compute hydrodynamic interactions between mono-disperse finite-size spherical particles in a pairwise fashion. The interactions have 2 components. The first is Ball-Melrose lubrication terms via the formulas in *(Ball and Melrose)*

$$W = -a_{sq}|(v_1 - v_2) \bullet \mathbf{nn}|^2 - a_{sh}|(\omega_1 + \omega_2) \bullet (\mathbf{I} - \mathbf{nn}) - 2\Omega_N|^2 - \\ a_{pu}|(\omega_1 - \omega_2) \bullet (\mathbf{I} - \mathbf{nn})|^2 - a_{tw}|(\omega_1 - \omega_2) \bullet \mathbf{nn}|^2 \qquad r < r_c$$

$$\Omega_N = \mathbf{n} \times (v_1 - v_2)/r$$

which represents the dissipation W between two nearby particles due to their relative velocities in the presence of a background solvent with viscosity *mu*. Note that this is dynamic viscosity which has units of mass/distance/time, not kinematic viscosity.

The Asq (squeeze) term is the strongest and is included if *flagHI* is set to 1 (default). It scales as 1/gap where gap is the separation between the surfaces of the 2 particles. The Ash (shear) and Apu (pump) terms are only included if *flaglog* is set to 1. They are the next strongest interactions, and the only other singular interaction, and scale as log(gap). Note that *flaglog* = 1 and *flagHI* = 0 is invalid, and will result in a warning message, after which *flagHI* will be set to 1. The Atw (twist) term is currently not included. It is typically a very small contribution to the lubrication forces.

The *flagHI* and *flagVF* settings are optional. Neither should be used, or both must be defined.

Cutinner sets the minimum center-to-center separation that will be used in calculations irrespective of the actual separation. *Cutoff* is the maximum center-to-center separation at which an interaction is computed. Using a *cutoff* less than 3 radii is recommended if *flaglog* is set to 1.

The other component is due to the Fast Lubrication Dynamics (FLD) approximation, described in *(Kumar)*, which can be represented by the following equation

$$F^H = -R_{FU}(U - U^\infty) + R_{FE}E^\infty$$

where U represents the velocities and angular velocities of the particles, U^∞ represents the velocity and the angular velocity of the undisturbed fluid, and E^∞ represents the rate of strain tensor of the undisturbed fluid with viscosity *mu*. Again, note that this is dynamic viscosity which has units of mass/distance/time, not kinematic viscosity. Volume fraction corrections to R_FU are included as long as *flagVF* is set to 1 (default).

Note: When using the FLD terms, these pair styles are designed to be used with explicit time integration and a correspondingly small timestep. Thus either *fix nve/sphere* or *fix nve/asphere* should be used for time integration. To perform implicit FLD, see the *pair_style lubricateU* command.

Style *lubricate* requires monodisperse spherical particles; style *lubricate/poly* allows for polydisperse spherical particles.

The viscosity *mu* can be varied in a time-dependent manner over the course of a simulation, in which case in which case the pair_style setting for *mu* will be overridden. See the *fix adapt* command for details.

If the suspension is sheared via the *fix deform* command then the pair style uses the shear rate to adjust the hydrodynamic interactions accordingly. Volume changes due to fix deform are accounted for when computing the volume fraction corrections to R_FU.

When computing the volume fraction corrections to R_FU, the presence of walls (whether moving or stationary) will affect the volume fraction available to colloidal particles. This is currently accounted for with the following types of walls: *wall/lj93*, *wall/lj126*, *wall/colloid*, and *wall/harmonic*. For these wall styles, the correct volume fraction will be used when walls do not coincide with the box boundary, as well as when walls move and thereby cause a change in the volume fraction. Other wall styles will still work, but they will result in the volume fraction being computed based on the box boundaries.

Since lubrication forces are dissipative, it is usually desirable to thermostat the system at a constant temperature. If Brownian motion (at a constant temperature) is desired, it can be set using the *pair_style brownian* command. These pair styles and the brownian style should use consistent parameters for *mu*, *flaglog*, *flagfld*, *cutinner*, *cutoff*, *flagHI* and *flagVF*.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- cutinner (distance units)
- cutoff (distance units)

The two coefficients are optional. If neither is specified, the two cutoffs specified in the pair_style command are used. Otherwise both must be specified.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in *this section* of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See *this section* of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the two cutoff distances for this pair style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style does not support the *pair_modify* shift option for the energy of the pair interaction.

The *pair_modify* table option is not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.311.3 Restrictions

These styles are part of the COLLOID package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Only spherical monodisperse particles are allowed for pair_style lubricate.

Only spherical particles are allowed for pair_style lubricate/poly.

These pair styles will not restart exactly when using the *read_restart* command, though they should provide statistically similar results. This is because the forces they compute depend on atom velocities. See the *read_restart* command for more details.

18.311.4 Related commands

pair_coeff, *pair_style lubricateU*

18.311.5 Default

The default settings for the optional args are flagHI = 1 and flagVF = 1.

(Ball) Ball and Melrose, Physica A, 247, 444-472 (1997).

(Kumar) Kumar and Higdon, Phys Rev E, 82, 051401 (2010). See also his thesis for more details: A. Kumar, "Microscale Dynamics in Suspensions of Non-spherical Particles", Thesis, University of Illinois Urbana-Champaign, (2010). (https://www.ideals.illinois.edu/handle/2142/16032)

18.312 pair_style lubricateU command

18.313 pair_style lubricateU/poly command

18.313.1 Syntax

```
pair_style style mu flaglog cutinner cutoff gdot flagHI flagVF
```

- style = *lubricateU* or *lubricateU/poly*

- mu = dynamic viscosity (dynamic viscosity units)
- flaglog = 0/1 to exclude/include log terms in the lubrication approximation
- cutinner = inner cut off distance (distance units)
- cutoff = outer cutoff for interactions (distance units)
- gdot = shear rate (1/time units)
- flagHI (optional) = 0/1 to exclude/include 1/r hydrodynamic interactions
- flagVF (optional) = 0/1 to exclude/include volume fraction corrections in the long-range isotropic terms

Examples: (all assume radius = 1)

```
pair_style lubricateU 1.5 1 2.01 2.5 0.01 1 1
pair_coeff 1 1 2.05 2.8
pair_coeff * *
```

18.313.2 Description

Styles *lubricateU* and *lubricateU/poly* compute velocities and angular velocities for finite-size spherical particles such that the hydrodynamic interaction balances the force and torque due to all other types of interactions.

The interactions have 2 components. The first is Ball-Melrose lubrication terms via the formulas in *(Ball and Melrose)*

$$W = -a_{sq}|(v_1 - v_2) \bullet \mathbf{nn}|^2 - a_{sh}|(\omega_1 + \omega_2) \bullet (\mathbf{I} - \mathbf{nn}) - 2\Omega_N|^2 - \\ a_{pu}|(\omega_1 - \omega_2) \bullet (\mathbf{I} - \mathbf{nn})|^2 - a_{tw}|(\omega_1 - \omega_2) \bullet \mathbf{nn}|^2 \qquad r < r_c$$

$$\Omega_N = \mathbf{n} \times (v_1 - v_2)/r$$

which represents the dissipation W between two nearby particles due to their relative velocities in the presence of a background solvent with viscosity *mu*. Note that this is dynamic viscosity which has units of mass/distance/time, not kinematic viscosity.

The Asq (squeeze) term is the strongest and is included as long as *flagHI* is set to 1 (default). It scales as 1/gap where gap is the separation between the surfaces of the 2 particles. The Ash (shear) and Apu (pump) terms are only included if *flaglog* is set to 1. They are the next strongest interactions, and the only other singular interaction, and scale as log(gap). Note that *flaglog* = 1 and *flagHI* = 0 is invalid, and will result in a warning message, after which *flagHI* will be set to 1. The Atw (twist) term is currently not included. It is typically a very small contribution to the lubrication forces.

The *flagHI* and *flagVF* settings are optional. Neither should be used, or both must be defined.

Cutinner sets the minimum center-to-center separation that will be used in calculations irrespective of the actual separation. *Cutoff* is the maximum center-to-center separation at which an interaction is computed. Using a *cutoff* less than 3 radii is recommended if *flaglog* is set to 1.

The other component is due to the Fast Lubrication Dynamics (FLD) approximation, described in *(Kumar)*. The equation being solved to balance the forces and torques is

$$-R_{FU}(U - U^\infty) = -R_{FE}E^\infty - F^{rest}$$

where U represents the velocities and angular velocities of the particles, U^∞ represents the velocities and the angular velocities of the undisturbed fluid, and E^∞ represents the rate of strain tensor of the undisturbed fluid flow with viscosity *mu*. Again, note that this is dynamic viscosity which has units of mass/distance/time, not kinematic viscosity. Volume fraction corrections to R_FU are included if *flagVF* is set to 1 (default).

F*rest* represents the forces and torques due to all other types of interactions, e.g. Brownian, electrostatic etc. Note that this algorithm neglects the inertial terms, thereby removing the restriction of resolving the small interial time scale, which may not be of interest for colloidal particles. This pair style solves for the velocity such that the hydrodynamic force balances all other types of forces, thereby resulting in a net zero force (zero inertia limit). When defining this pair style, it must be defined last so that when this style is invoked all other types of forces have already been computed. For the same reason, it won't work if additional non-pair styles are defined (such as bond or Kspace forces) as they are calculated in LAMMPS after the pairwise interactions have been computed.

Note: When using these styles, the these pair styles are designed to be used with implicit time integration and a correspondingly larger timestep. Thus either *fix nve/noforce* should be used for spherical particles defined via *atom_style sphere* or *fix nve/asphere/noforce* should be used for spherical particles defined via *atom_style ellipsoid*. This is because the velocity and angular momentum of each particle is set by the pair style, and should not be reset by the time integration fix.

Style *lubricateU* requires monodisperse spherical particles; style *lubricateU/poly* allows for polydisperse spherical particles.

If the suspension is sheared via the *fix deform* command then the pair style uses the shear rate to adjust the hydrodynamic interactions accordingly. Volume changes due to fix deform are accounted for when computing the volume fraction corrections to R_FU.

When computing the volume fraction corrections to R_FU, the presence of walls (whether moving or stationary) will affect the volume fraction available to colloidal particles. This is currently accounted for with the following types of walls: *wall/lj93*, *wall/lj126*, *wall/colloid*, and *wall/harmonic*. For these wall styles, the correct volume fraction will be used when walls do not coincide with the box boundary, as well as when walls move and thereby cause a change in the volume fraction. To use these wall styles with pair_style *lubricateU* or *lubricateU/poly*, the *fld yes* option must be specified in the fix wall command.

Since lubrication forces are dissipative, it is usually desirable to thermostat the system at a constant temperature. If Brownian motion (at a constant temperature) is desired, it can be set using the *pair_style brownian* command. These pair styles and the brownian style should use consistent parameters for *mu*, *flaglog*, *flagfld*, *cutinner*, *cutoff*, *flagHI* and *flagVF*.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- cutinner (distance units)
- cutoff (distance units)

The two coefficients are optional. If neither is specified, the two cutoffs specified in the pair_style command are used. Otherwise both must be specified.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the two cutoff distances for this pair style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style does not support the *pair_modify* shift option for the energy of the pair interaction.

The *pair_modify* table option is not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.313.3 Restrictions

These styles are part of the COLLOID package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Currently, these pair styles assume that all other types of forces/torques on the particles have been already been computed when it is invoked. This requires this style to be defined as the last of the pair styles, and that no fixes apply additional constraint forces. One exception is the *fix wall/colloid* commands, which has an "fld" option to apply their wall forces correctly.

Only spherical monodisperse particles are allowed for pair_style lubricateU.

Only spherical particles are allowed for pair_style lubricateU/poly.

For sheared suspensions, it is assumed that the shearing is done in the xy plane, with x being the velocity direction and y being the velocity-gradient direction. In this case, one must use *fix deform* with the same rate of shear (erate).

18.313.4 Related commands

pair_coeff, *pair_style lubricate*

18.313.5 Default

The default settings for the optional args are flagHI = 1 and flagVF = 1.

(Ball) Ball and Melrose, Physica A, 247, 444-472 (1997).

(Kumar) Kumar and Higdon, Phys Rev E, 82, 051401 (2010).

18.314 pair_style lj/mdf command

18.315 pair_style buck/mdf command

18.316 pair_style lennard/mdf command

18.316.1 Syntax

```
pair_style style args
```

- style = *lj/mdf* or *buck/mdf* or *lennard/mdf*
- args = list of arguments for a particular style

```
lj/mdf args = cutoff1 cutoff2
  cutoff1 = inner cutoff for the start of the tapering function
  cutoff1 = out cutoff for the end of the tapering function
buck/mdf args = cutoff1 cutoff2
  cutoff1 = inner cutoff for the start of the tapering function
  cutoff1 = out cutoff for the end of the tapering function
lennard/mdf args = cutoff1 cutoff2
  cutoff1 = inner cutoff for the start of the tapering function
  cutoff1 = out cutoff for the end of the tapering function
```

18.316.2 Examples

```
pair_style lj/mdf 2.5 3.0
pair_coeff * * 1.0 1.0
pair_coeff 1 1 1.1 2.8 3.0 3.2

pair_style buck 2.5 3.0
pair_coeff * * 100.0 1.5 200.0
pair_coeff * * 100.0 1.5 200.0 3.0 3.5

pair_style lennard/mdf 2.5 3.0
pair_coeff * * 1.0 1.0
pair_coeff 1 1 1021760.3664 2120.317338 3.0 3.2
```

18.316.3 Description

The *lj/mdf*, *buck/mdf* and *lennard/mdf* compute the standard 12-6 Lennard-Jones and Buckingham potential with the addition of a taper function that ramps the energy and force smoothly to zero between an inner and outer cutoff.

$$E_{smooth}(r) = E(r) * f(r)$$

The tapering, *f(r)*, is done by using the Mei, Davenport, Fernando function *(Mei)*.

$$\begin{aligned} f(r) &= 1.0 && \text{for} \quad r < r_m \\ f(r) &= (1-x)^3 * (1+3x+6x^2) && \text{for} \quad r_m < r < r_{cut} \\ f(r) &= 0.0 && \text{for} \quad r >= r_{cut} \end{aligned}$$

where

$$x = \frac{(r - r_m)}{(r_{cut} - r_m)}$$

Here r_m is the inner cutoff radius and r_{cut} is the outer cutoff radius.

For the *lj/mdf* pair_style, the potential energy, *E(r)*, is the standard 12-6 Lennard-Jones written in the epsilon/sigma form:

$$E(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

Either the first two or all of the following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file read by the *read_data*. The two cutoffs default to the global values and ϵ and σ can also be determined by mixing as described below:

- ϵ (energy units)
- σ (distance units)
- r_m (distance units)
- r_{cut} (distance units)

For the *buck/mdf* pair_style, the potential energy, *E(r)*, is the standard Buckingham potential with three required coefficients. The two cutoffs can be omitted and default to the corresponding global values:

$$E(r) = Ae^{(-r/\rho)} - \frac{C}{r^6}$$

- *A* (energy units)
- ρ (distance units)
- *C* (energy-distance^6 units)
- r_m (distance units)
- r_{cut} (distance units)

For the *lennard/mdf* pair_style, the potential energy, *E(r)*, is the standard 12-6 Lennard-Jones written in the A/B form:

$$E(r) = \frac{A}{r^{12}} - \frac{B}{r^6}$$

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file read by the read_data commands, or by mixing as described below. The two cutoffs default to their global values and must be either both given or both left out:

- *A* (energy-distance^12 units)
- *B* (energy-distance^6 units)
- r_m (distance units)
- r_{cut} (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the ϵ and $sigma$ coefficients and cutoff distances for the lj/mdf pair style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details. The other two pair styles buck/mdf and lennard/mdf do not support mixing, so all I,J pairs of coefficients must be specified explicitly.

None of the lj/mdf, buck/mdf, or lennard/mdf pair styles supports the *pair_modify* shift option or long-range tail corrections to pressure and energy.

These styles write their information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These styles can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

18.316.4 Restrictions

These pair styles can only be used if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

18.316.5 Related commands

pair_coeff

Default: none

(Mei) Mei, Davenport, Fernando, Phys Rev B, 43 4653 (1991)

18.317 pair_style meam/spline command

18.318 pair_style meam/spline/omp command

18.318.1 Syntax

```
pair_style meam/spline
```

18.318.2 Examples

```
pair_style meam/spline
pair_coeff * * Ti.meam.spline Ti
pair_coeff * * Ti.meam.spline Ti Ti Ti
```

18.318.3 Description

The *meam/spline* style computes pairwise interactions for metals using a variant of modified embedded-atom method (MEAM) potentials *(Lenosky)*. For a single species ("old-style") MEAM, the total energy E is given by

$$E = \sum_{i<j} \phi(r_{ij}) + \sum_i U(n_i)$$
$$n_i = \sum_j \rho(r_{ij}) + \sum_{\substack{j<k,\\ j,k\neq i}} f(r_{ij}) f(r_{ik}) g[\cos(\theta_{jik})]$$

where ρ_i is the density at atom I, θ_{jik} is the angle between atoms J, I, and K centered on atom I. The five functions ϕ, U, ρ, f, and g are represented by cubic splines.

The *meam/spline* style also supports a new style multicomponent modified embedded-atom method (MEAM) potential *(Zhang)*, where the total energy E is given by

$$E = \sum_{i<j} \phi_{ij}(r_{ij}) + \sum_i U_i(n_i)$$
$$n_i = \sum_{j\neq i} \rho_j(r_{ij}) + \sum_{\substack{j<k,\\ j,k\neq i}} f_j(r_{ij}) f_k(r_{ik}) g_{jk}[\cos(\theta_{jik})]$$

where the five functions ϕ, U, ρ, f, and g depend on the chemistry of the atoms in the interaction. In particular, if there are N different chemistries, there are N different U, ρ, and f functions, while there are N(N+1)/2 different ϕ and g functions. The new style multicomponent MEAM potential files are indicated by the second line in the file starts with "meam/spline" followed by the number of elements and the name of each element.

The cutoffs and the coefficients for these spline functions are listed in a parameter file which is specified by the *pair_coeff* command. Parameter files for different elements are included in the "potentials" directory of the LAMMPS distribution and have a ".meam.spline" file suffix. All of these files are parameterized in terms of LAMMPS *metal units*.

Note that unlike for other potentials, cutoffs for spline-based MEAM potentials are not set in the pair_style or pair_coeff command; they are specified in the potential files themselves.

Unlike the EAM pair style, which retrieves the atomic mass from the potential file, the spline-based MEAM potentials do not include mass information; thus you need to use the *mass* command to specify it.

Only a single pair_coeff command is used with the *meam/spline* style which specifies a potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of spline-based MEAM elements to atom types

See the *pair_coeff* doc page for alternate ways to specify the path for the potential file.

As an example, imagine the Ti.meam.spline file has values for Ti (old style). If your LAMMPS simulation has 3 atoms types and they are all to be treated with this potentials, you would use the following pair_coeff command:

```
pair_coeff * * Ti.meam.spline Ti Ti Ti
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The three Ti arguments map LAMMPS atom types 1,2,3 to the Ti element in the potential file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *meam/spline* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials. The old-style potential maps any non-NULL species named on the command line to that single type.

An example with a two component spline (new style) is TiO.meam.spline, where the command

```
pair_coeff * * TiO.meam.spline Ti O
```

will map the 1st atom type to Ti and the second atom type to O. Note in this case that the species names need to match exactly with the names of the elements in the TiO.meam.spline file; otherwise an error will be raised. This behavior is different than the old style MEAM files.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the *pair_modify* shift, table, and tail options.

The *meam/spline* pair style does not write its information to *binary restart files*, since it is stored in an external potential parameter file. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

The *meam/spline* pair style can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

18.318.4 Restrictions

This pair style requires the *newton* setting to be "on" for pair interactions.

This pair style is only enabled if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

18.318.5 Related commands

pair_coeff, *pair_style meam/c*

Default: none

(Lenosky) Lenosky, Sadigh, Alonso, Bulatov, de la Rubia, Kim, Voter, Kress, Modelling Simulation Materials Science Engineering, 8, 825 (2000).

(Zhang) Zhang and Trinkle, Computational Materials Science, 124, 204-210 (2016).

18.319 pair_style meam/sw/spline command

18.319.1 Syntax

```
pair_style meam/sw/spline
```

18.319.2 Examples

```
pair_style meam/sw/spline
pair_coeff * * Ti.meam.sw.spline Ti
pair_coeff * * Ti.meam.sw.spline Ti Ti Ti
```

18.319.3 Description

The *meam/sw/spline* style computes pairwise interactions for metals using a variant of modified embedded-atom method (MEAM) potentials *(Lenosky)* with an additional Stillinger-Weber (SW) term *(Stillinger)* in the energy. This form of the potential was first proposed by Nicklas, Fellinger, and Park *(Nicklas)*. We refer to it as MEAM+SW. The total energy E is given by

$$
\begin{aligned}
E &= E_{MEAM} + E_{SW} \\
E_{MEAM} &= \sum_{IJ} \phi(r_{IJ}) + \sum_{I} U(\rho_I) \\
E_{SW} &= \sum_{I} \sum_{JK} F(r_{IJ})\, F(r_{IK})\, G(\cos(\theta_{JIK})) \\
\rho_I &= \sum_{J} \rho(r_{IJ}) + \sum_{JK} f(r_{IJ})\, f(r_{IK})\, g(\cos(\theta_{JIK}))
\end{aligned}
$$

where ρ_I is the density at atom I, θ_{JIK} is the angle between atoms J, I, and K centered on atom I. The seven functions ϕ, F, G, U, ρ, f, and g are represented by cubic splines.

The cutoffs and the coefficients for these spline functions are listed in a parameter file which is specified by the *pair_coeff* command. Parameter files for different elements are included in the "potentials" directory of the LAMMPS distribution and have a ".meam.sw.spline" file suffix. All of these files are parameterized in terms of LAMMPS *metal units*.

Note that unlike for other potentials, cutoffs for spline-based MEAM+SW potentials are not set in the pair_style or pair_coeff command; they are specified in the potential files themselves.

Unlike the EAM pair style, which retrieves the atomic mass from the potential file, the spline-based MEAM+SW potentials do not include mass information; thus you need to use the *mass* command to specify it.

Only a single pair_coeff command is used with the meam/sw/spline style which specifies a potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of spline-based MEAM+SW elements to atom types

See the *pair_coeff* doc page for alternate ways to specify the path for the potential file.

As an example, imagine the Ti.meam.sw.spline file has values for Ti. If your LAMMPS simulation has 3 atoms types and they are all to be treated with this potential, you would use the following pair_coeff command:

pair_coeff * * Ti.meam.sw.spline Ti Ti Ti

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The three Ti arguments map LAMMPS atom types 1,2,3 to the Ti element in the potential file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *meam/sw/spline* potential is used as part of the hybrid pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Note: The *meam/sw/spline* style currently supports only single-element MEAM+SW potentials. It may be extended for alloy systems in the future.

Example input scripts that use this pair style are provided in the examples/USER/misc/meam_sw_spline directory.

Mixing, shift, table, tail correction, restart, rRESPA info:

The pair style does not support multiple element types or mixing. It has been designed for pure elements only.

This pair style does not support the *pair_modify* shift, table, and tail options.

The *meam/sw/spline* pair style does not write its information to *binary restart files*, since it is stored in an external potential parameter file. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

The *meam/sw/spline* pair style can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

18.319.4 Restrictions

This pair style requires the *newton* setting to be "on" for pair interactions.

This pair style is only enabled if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

18.319.5 Related commands

pair_coeff, *pair_style meam/c*, *pair_style meam/spline*

Default: none

(Lenosky) Lenosky, Sadigh, Alonso, Bulatov, de la Rubia, Kim, Voter, Kress, Modell. Simul. Mater. Sci. Eng. 8, 825 (2000).

(Stillinger) Stillinger, Weber, Phys. Rev. B 31, 5262 (1985).

(Nicklas) The spline-based MEAM+SW format was first devised and used to develop potentials for bcc transition metals by Jeremy Nicklas, Michael Fellinger, and Hyoungki Park at The Ohio State University.

18.320 pair_style meam/c command

18.320.1 Syntax

```
pair_style meam/c
```

18.320.2 Examples

```
pair_style meam/c
pair_coeff * * ../potentials/library.meam Si ../potentials/si.meam Si
pair_coeff * * ../potentials/library.meam Ni Al NULL Ni Al Ni Ni
```

18.320.3 Description

Note: The behavior of the MEAM potential for alloy systems has changed as of November 2010; see description below of the mixture_ref_t parameter

Style *meam/c* computes pairwise interactions for a variety of materials using modified embedded-atom method (MEAM) potentials *(Baskes)*. Conceptually, it is an extension to the original *EAM potentials* which adds angular forces. It is thus suitable for modeling metals and alloys with fcc, bcc, hcp and diamond cubic structures, as well as covalently bonded materials like silicon and carbon. Style *meam/c* is a translation of the (now obsolete) *meam* code from Fortran to C++. It is functionally equivalent to *meam* but more efficient, and thus *meam* has been removed from LAMMPS after the 12 December 2018 release.

In the MEAM formulation, the total energy E of a system of atoms is given by:

$$E = \sum_i \left\{ F_i(\bar{\rho}_i) + \frac{1}{2} \sum_{i \neq j} \phi_{ij}(r_{ij}) \right\}$$

where F is the embedding energy which is a function of the atomic electron density ρ, and ϕ is a pair potential interaction. The pair interaction is summed over all neighbors J of atom I within the cutoff distance. As with EAM, the multi-body nature of the MEAM potential is a result of the embedding energy term. Details of the computation of the embedding and pair energies, as implemented in LAMMPS, are given in *(Gullet)* and references therein.

The various parameters in the MEAM formulas are listed in two files which are specified by the *pair_coeff* command. These are ASCII text files in a format consistent with other MD codes that implement MEAM potentials, such as the serial DYNAMO code and Warp. Several MEAM potential files with parameters for different materials are included in the "potentials" directory of the LAMMPS distribution with a ".meam" suffix. All of these are parameterized in terms of LAMMPS *metal units*.

Note that unlike for other potentials, cutoffs for MEAM potentials are not set in the pair_style or pair_coeff command; they are specified in the MEAM potential files themselves.

Only a single pair_coeff command is used with the *meam* style which specifies two MEAM files and the element(s) to extract information for. The MEAM elements are mapped to LAMMPS atom types by specifying N additional arguments after the 2nd filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- MEAM library file
- Elem1, Elem2, ...
- MEAM parameter file
- N element names = mapping of MEAM elements to atom types

See the *pair_coeff* doc page for alternate ways to specify the path for the potential files.

As an example, the potentials/library.meam file has generic MEAM settings for a variety of elements. The potentials/SiC.meam file has specific parameter settings for a Si and C alloy system. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * library.meam Si C sic.meam Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The two filenames are for the library and parameter file respectively. The Si and C arguments (between the file names) are the two elements for which info will be extracted from the library file. The first three trailing Si arguments map LAMMPS atom types 1,2,3 to the MEAM Si element. The final C argument maps LAMMPS atom type 4 to the MEAM C element.

If the 2nd filename is specified as NULL, no parameter file is read, which simply means the generic parameters in the library file are used. Use of the NULL specification for the parameter file is discouraged for systems with more than

a single element type (e.g. alloys), since the parameter file is expected to set element interaction terms that are not captured by the information in the library file.

If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *meam* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Note: If the 2nd filename is NULL, the element names between the two filenames can appear in any order, e.g. "Si C" or "C Si" in the example above. However, if the 2nd filename is not NULL (as in the example above), it contains settings that are Fortran-indexed for the elements that preceed it. Thus you need to insure you list the elements between the filenames in an order consistent with how the values in the 2nd filename are indexed. See details below on the syntax for settings in the 2nd file.

The MEAM library file provided with LAMMPS has the name potentials/library.meam. It is the "meamf" file used by other MD codes. Aside from blank and comment lines (start with #) which can appear anywhere, it is formatted as a series of entries, each of which has 19 parameters and can span multiple lines:

elt, lat, z, ielement, atwt, alpha, b0, b1, b2, b3, alat, esub, asub, t0, t1, t2, t3, rozero, ibar

The "elt" and "lat" parameters are text strings, such as elt = Si or Cu and lat = dia or fcc. Because the library file is used by Fortran MD codes, these strings may be enclosed in single quotes, but this is not required. The other numeric parameters match values in the formulas above. The value of the "elt" string is what is used in the pair_coeff command to identify which settings from the library file you wish to read in. There can be multiple entries in the library file with the same "elt" value; LAMMPS reads the 1st matching entry it finds and ignores the rest.

Other parameters in the MEAM library file correspond to single-element potential parameters:

```
lat      = lattice structure of reference configuration
z        = number of nearest neighbors in the reference structure
ielement = atomic number
atwt     = atomic weight
alat     = lattice constant of reference structure
esub     = energy per atom (eV) in the reference structure at equilibrium
asub     = "A" parameter for MEAM (see e.g. (Baskes))
```

The alpha, b0, b1, b2, b3, t0, t1, t2, t3 parameters correspond to the standard MEAM parameters in the literature *(Baskes)* (the b parameters are the standard beta parameters). Note that only parameters normalized to t0 = 1.0 are supported. The rozero parameter is an element-dependent density scaling that weights the reference background density (see e.g. equation 4.5 in *(Gullet)*) and is typically 1.0 for single-element systems. The ibar parameter selects the form of the function G(Gamma) used to compute the electron density; options are

```
 0 => G = sqrt(1+Gamma)
 1 => G = exp(Gamma/2)
 2 => not implemented
 3 => G = 2/(1+exp(-Gamma))
 4 => G = sqrt(1+Gamma)
-5 => G = +-sqrt(abs(1+Gamma))
```

If used, the MEAM parameter file contains settings that override or complement the library file settings. Examples of such parameter files are in the potentials directory with a ".meam" suffix. Their format is the same as is read by other Fortran MD codes. Aside from blank and comment lines (start with #) which can appear anywhere, each line has one of the following forms. Each line can also have a trailing comment (starting with #) which is ignored.

```
keyword = value
keyword(I) = value
keyword(I,J) = value
keyword(I,J,K) = value
```

The indices I, J, K correspond to the elements selected from the MEAM library file numbered in the order of how those elements were selected starting from 1. Thus for the example given below

```
pair_coeff * * library.meam Si C sic.meam Si Si Si C
```

an index of 1 would refer to Si and an index of 2 to C.

The recognized keywords for the parameter file are as follows:

Ec, alpha, rho0, delta, lattce, attrac, repuls, nn2, Cmin, Cmax, rc, delr, augt1, gsmooth_factor, re

where

```
rc          = cutoff radius for cutoff function; default = 4.0
delr        = length of smoothing distance for cutoff function; default = 0.1
rho0(I)     = relative density for element I (overwrites value
              read from meamf file)
Ec(I,J)     = cohesive energy of reference structure for I-J mixture
delta(I,J)  = heat of formation for I-J alloy; if Ec_IJ is input as
              zero, then LAMMPS sets Ec_IJ = (Ec_II + Ec_JJ)/2 - delta_IJ
alpha(I,J)  = alpha parameter for pair potential between I and J (can
              be computed from bulk modulus of reference structure
re(I,J)     = equilibrium distance between I and J in the reference
              structure
Cmax(I,J,K) = Cmax screening parameter when I-J pair is screened
              by K (I<=J); default = 2.8
Cmin(I,J,K) = Cmin screening parameter when I-J pair is screened
              by K (I<=J); default = 2.0
lattce(I,J) = lattice structure of I-J reference structure:
                fcc = face centered cubic
                bcc = body centered cubic
                hcp = hexagonal close-packed
                dim = dimer
                dia = diamond (interlaced fcc for alloy)
                dia3= diamond structure with primary 1NN and secondary 3NN␣
↪interation
                b1  = rock salt (NaCl structure)
                c11 = MoSi2 structure
                l12 = Cu3Au structure (lower case L, followed by 12)
                b2  = CsCl structure (interpenetrating simple cubic)
                ch4 = methane-like structure, only for binary system
                lin = linear structure (180 degree angle)
                zig = zigzag structure with a uniform angle
                tri = H2O-like structure that has an angle
nn2(I,J)    = turn on second-nearest neighbor MEAM formulation for
              I-J pair (see for example (Lee)).
                0 = second-nearest neighbor formulation off
                1 = second-nearest neighbor formulation on
                default = 0
attrac(I,J) = additional cubic attraction term in Rose energy I-J pair␣
↪potential
                default = 0
repuls(I,J) = additional cubic repulsive term in Rose energy I-J pair␣
↪potential
                default = 0
zbl(I,J)    = blend the MEAM I-J pair potential with the ZBL potential for␣
```

```
↪small
              atom separations (ZBL)
                default = 1
theta(I,J)  = angle between three atoms in line, zigzag, and trimer reference␣
↪structures in degrees
                default = 180
gsmooth_factor  = factor determining the length of the G-function smoothing
                  region; only significant for ibar=0 or ibar=4.
                      99.0 = short smoothing region, sharp step
                      0.5  = long smoothing region, smooth step
                      default = 99.0
augt1           = integer flag for whether to augment t1 parameter by
                  3/5*t3 to account for old vs. new meam formulations;
                    0 = don't augment t1
                    1 = augment t1
                    default = 1
ialloy          = integer flag to use alternative averaging rule for t␣
↪parameters,
                  for comparison with the DYNAMO MEAM code
                    0 = standard averaging (matches ialloy=0 in DYNAMO)
                    1 = alternative averaging (matches ialloy=1 in DYNAMO)
                    2 = no averaging of t (use single-element values)
                    default = 0
mixture_ref_t   = integer flag to use mixture average of t to compute the␣
↪background
                  reference density for alloys, instead of the single-element␣
↪values
                  (see description and warning elsewhere in this doc page)
                    0 = do not use mixture averaging for t in the reference␣
↪density
                    1 = use mixture averaging for t in the reference density
                    default = 0
erose_form      = integer value to select the form of the Rose energy function
                  (see description below).
                    default = 0
emb_lin_neg     = integer value to select embedding function for negative␣
↪densities
                    0 = F(rho)=0
                    1 = F(rho) = -asub*esub*rho (linear in rho, matches␣
↪DYNAMO)
                    default = 0
bkgd_dyn        = integer value to select background density formula
                    0 = rho_bkgd = rho_ref_meam(a) (as in the reference␣
↪structure)
                    1 = rho_bkgd = rho0_meam(a)*Z_meam(a) (matches DYNAMO)
                    default = 0
```

Rc, delr, re are in distance units (Angstroms in the case of metal units). Ec and delta are in energy units (eV in the case of metal units).

Each keyword represents a quantity which is either a scalar, vector, 2d array, or 3d array and must be specified with the correct corresponding array syntax. The indices I,J,K each run from 1 to N where N is the number of MEAM elements being used.

Thus these lines

```
rho0(2) = 2.25
alpha(1,2) = 4.37
```

set rho0 for the 2nd element to the value 2.25 and set alpha for the alloy interaction between elements 1 and 2 to 4.37.

The augt1 parameter is related to modifications in the MEAM formulation of the partial electron density function. In recent literature, an extra term is included in the expression for the third-order density in order to make the densities orthogonal (see for example *(Wang)*, equation 3d); this term is included in the MEAM implementation in lammps. However, in earlier published work this term was not included when deriving parameters, including most of those provided in the library.meam file included with lammps, and to account for this difference the parameter t1 must be augmented by 3/5*t3. If augt1=1, the default, this augmentation is done automatically. When parameter values are fit using the modified density function, as in more recent literature, augt1 should be set to 0.

The mixture_ref_t parameter is available to match results with those of previous versions of lammps (before January 2011). Newer versions of lammps, by default, use the single-element values of the t parameters to compute the background reference density. This is the proper way to compute these parameters. Earlier versions of lammps used an alloy mixture averaged value of t to compute the background reference density. Setting mixture_ref_t=1 gives the old behavior. WARNING: using mixture_ref_t=1 will give results that are demonstrably incorrect for second-neighbor MEAM, and non-standard for first-neighbor MEAM; this option is included only for matching with previous versions of lammps and should be avoided if possible.

The parameters attrac and repuls, along with the integer selection parameter erose_form, can be used to modify the Rose energy function used to compute the pair potential. This function gives the energy of the reference state as a function of interatomic spacing. The form of this function is:

```
astar = alpha * (r/re - 1.d0)
if erose_form = 0: erose = -Ec*(1+astar+a3*(astar**3)/(r/re))*exp(-astar)
if erose_form = 1: erose = -Ec*(1+astar+(-attrac+repuls/r)*(astar**3))*exp(-astar)
if erose_form = 2: erose = -Ec*(1 +astar + a3*(astar**3))*exp(-astar)
a3 = repuls, astar < 0
a3 = attrac, astar >= 0
```

Most published MEAM parameter sets use the default values attrac=repulse=0. Setting repuls=attrac=delta corresponds to the form used in several recent published MEAM parameter sets, such as *(Valone)*

Note: The default form of the erose expression in LAMMPS was corrected in March 2009. The current version is correct, but may show different behavior compared with earlier versions of lammps with the attrac and/or repuls parameters are non-zero. To obtain the previous default form, use erose_form = 1 (this form does not seem to appear in the literature). An alternative form (see e.g. *(Lee2)*) is available using erose_form = 2.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS with user-specifiable parameters as described above. You never need to specify a pair_coeff command with I != J arguments for this style.

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.320.4 Restrictions

The *meam/c* style is provided in the USER-MEAMC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

The maximum number of elements, that can be read from the MEAM library file, is determined at compile time. The default is 5. If you need support for more elements, you have to change the define for the constant 'maxelt' at the beginning of the file src/USER-MEAMC/meam.h and update/recompile LAMMPS. There is no limit on the number of atoms types.

18.320.5 Related commands

pair_coeff, *pair_style eam*, *pair_style meam/spline*

Default: none

(Baskes) Baskes, Phys Rev B, 46, 2727-2742 (1992).

(Gullet) Gullet, Wagner, Slepoy, SANDIA Report 2003-8782 (2003). This report may be accessed on-line via this link. **(Lee)** Lee, Baskes, Phys. Rev. B, 62, 8564-8567 (2000).

(Lee2) Lee, Baskes, Kim, Cho. Phys. Rev. B, 64, 184102 (2001).

(Valone) Valone, Baskes, Martin, Phys. Rev. B, 73, 214209 (2006).

(Wang) Wang, Van Hove, Ross, Baskes, J. Chem. Phys., 121, 5410 (2004).

(ZBL) J.F. Ziegler, J.P. Biersack, U. Littmark, "Stopping and Ranges of Ions in Matter", Vol 1, 1985, Pergamon Press.

18.321 pair_style edpd command

18.322 pair_style mdpd command

18.323 pair_style mdpd/rhosum command

18.324 pair_style tdpd command

18.324.1 Syntax

```
pair_style style args
```

- style = *edpd* or *mdpd* or *mdpd/rhosum* or *tdpd*
- args = list of arguments for a particular style

```
edpd args = cutoff seed
  cutoff = global cutoff for eDPD interactions (distance units)
  seed = random # seed (integer) (if <= 0, eDPD will use current time as␣
↪the seed)
mdpd args = T cutoff seed
  T = temperature (temperature units)
  cutoff = global cutoff for mDPD interactions (distance units)
```

```
    seed = random # seed (integer) (if <= 0, mDPD will use current time as␣
 ↪the seed)
  mdpd/rhosum args =
  tdpd args = T cutoff seed
    T = temperature (temperature units)
    cutoff = global cutoff for tDPD interactions (distance units)
    seed = random # seed (integer) (if <= 0, tDPD will use current time as␣
 ↪the seed)
```

18.324.2 Examples

```
pair_style edpd 1.58 9872598
pair_coeff * * 18.75 4.5 0.41 1.58 1.42E-5 2.0 1.58
pair_coeff 1 1 18.75 4.5 0.41 1.58 1.42E-5 2.0 1.58 power 10.54 -3.66 3.44 -4.10
pair_coeff 1 1 18.75 4.5 0.41 1.58 1.42E-5 2.0 1.58 power 10.54 -3.66 3.44 -4.10␣
↪kappa -0.44 -3.21 5.04 0.00

pair_style hybrid/overlay mdpd/rhosum mdpd 1.0 1.0 65689
pair_coeff 1 1 mdpd/rhosum  0.75
pair_coeff 1 1 mdpd -40.0 25.0 18.0 1.0 0.75

pair_style tdpd 1.0 1.58 935662
pair_coeff * * 18.75 4.5 0.41 1.58 1.58 1.0 1.0E-5 2.0
pair_coeff 1 1 18.75 4.5 0.41 1.58 1.58 1.0 1.0E-5 2.0 3.0 1.0E-5 2.0
```

18.324.3 Description

The *edpd* style computes the pairwise interactions and heat fluxes for eDPD particles following the formulations in *(Li2014_JCP)* and *Li2015_CC*. The time evolution of an eDPD particle is governed by the conservation of momentum and energy given by

$$\frac{\mathrm{d}^2\mathbf{r}_i}{\mathrm{d}t^2} = \frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = \mathbf{F}_i = \sum_{i\neq j}(\mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R)$$

$$C_v\frac{\mathrm{d}T_i}{\mathrm{d}t} = q_i = \sum_{i\neq j}(q_{ij}^C + q_{ij}^V + q_{ij}^R),$$

where the three components of F_i including the conservative force F_{ij}^C, dissipative force F_{ij}^D and random force F_{ij}^R are expressed as

$$\begin{aligned}
\mathbf{F}_{ij}^C &= \alpha_{ij}\omega_C(r_{ij})\mathbf{e}_{ij} \\
\mathbf{F}_{ij}^D &= -\gamma\omega_D(r_{ij})(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})\mathbf{e}_{ij} \\
\mathbf{F}_{ij}^R &= \sigma\omega_R(r_{ij})\xi_{ij}\Delta t^{-1/2}\mathbf{e}_{ij} \\
\omega_C(r) &= 1 - r/r_c \\
\alpha_{ij} &= A\cdot k_B(T_i + T_j)/2 \\
\omega_D(r) &= \omega_R^2(r) = (1 - r/r_c)^s \\
\sigma_{ij}^2 &= 4\gamma k_B T_i T_j/(T_i + T_j)
\end{aligned}$$

in which the exponent of the weighting function s can be defined as a temperature-dependent variable. The heat flux between particles accounting for the collisional heat flux q^C, viscous heat flux q^V, and random heat flux q^R are given

by

$$
\begin{aligned}
q_i^C &= \sum_{j \neq i} k_{ij} \omega_{CT}(r_{ij}) \left(\frac{1}{T_i} - \frac{1}{T_j} \right) \\
q_i^V &= \frac{1}{2C_v} \sum_{j \neq i} \left\{ \omega_D(r_{ij}) \left[\gamma_{ij} \left(\mathbf{e}_{ij} \cdot \mathbf{v}_{ij} \right)^2 - \frac{(\sigma_{ij})^2}{m} \right] - \sigma_{ij} \omega_R(r_{ij}) \left(\mathbf{e}_{ij} \cdot \mathbf{v}_{ij} \right) \xi_{ij} \right\} \\
q_i^R &= \sum_{j \neq i} \beta_{ij} \omega_{RT}(r_{ij}) dt^{-1/2} \xi_{ij}^e \\
\omega_{CT}(r) &= \omega_{RT}^2(r) = (1 - r/r_{ct})^{s_T} \\
k_{ij} &= C_v^2 \kappa (T_i + T_j)^2 / 4k_B \\
\beta_{ij}^2 &= 2k_B k_{ij}
\end{aligned}
$$

where the mesoscopic heat friction κ is given by

$$
\kappa = \frac{315 k_B \upsilon}{2\pi\rho C_v r_{ct}^5} \frac{1}{Pr},
$$

with υ being the kinematic viscosity. For more details, see Eq.(15) in *(Li2014_JCP)*.

The following coefficients must be defined in eDPD system for each pair of atom types via the *pair_coeff* command as in the examples above.

- A (force units)
- γ (force/velocity units)
- power_f (positive real)
- cutoff (distance units)
- kappa (thermal conductivity units)
- power_T (positive real)
- cutoff_T (distance units)
- optional keyword = power or kappa

The keyword *power* or *kappa* is optional. Both "power" and "kappa" require 4 parameters c_1, c_2, c_3, c_4 showing the temperature dependence of the exponent $s(T) = \text{power}_f(1 + c_1(T-1) + c_2(T-1)^2 + c_3(T-1)^3 + c_4(T-1)^4)$ and of the mesoscopic heat friction $s_T(T) = \kappa(1 + c_1(T-1) + c_2(T-1)^2 + c_3(T-1)^3 + c_4(T-1)^4)$. If the keyword *power* or *kappa* is not specified, the eDPD system will use constant power_f and κ, which is independent to temperature changes.

The *mdpd/rhosum* style computes the local particle mass density ρ for mDPD particles by kernel function interpolation.

The following coefficients must be defined for each pair of atom types via the *pair_coeff* command as in the examples above.

- cutoff (distance units)

The *mdpd* style computes the many-body interactions between mDPD particles following the formulations in *(Li2013_POF)*. The dissipative and random forces are in the form same as the classical DPD, but the conservative force is local density dependent, which are given by

$$
\begin{aligned}
\mathbf{F}_{ij}^C &= A w_c(r_{ij}) \mathbf{e}_{ij} + B(\rho_i + \rho_j) w_d(r_{ij}) \mathbf{e}_{ij} \\
\mathbf{F}_{ij}^D &= -\gamma \omega_D(r_{ij}) (\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}) \mathbf{e}_{ij} \\
\mathbf{F}_{ij}^R &= \sigma \omega_R(r_{ij}) \xi_{ij} \Delta t^{-1/2} \mathbf{e}_{ij}
\end{aligned}
$$

where the first term in F_C with a negative coefficient $A < 0$ stands for an attractive force within an interaction range r_c, and the second term with $B > 0$ is the density-dependent repulsive force within an interaction range r_d.

The following coefficients must be defined for each pair of atom types via the *pair_coeff* command as in the examples above.

- A (force units)
- B (force units)
- γ (force/velocity units)
- cutoff_c (distance units)
- cutoff_d (distance units)

The *tdpd* style computes the pairwise interactions and chemical concentration fluxes for tDPD particles following the formulations in *(Li2015_JCP)*. The time evolution of a tDPD particle is governed by the conservation of momentum and concentration given by

$$\frac{\mathrm{d}^2\mathbf{r}_i}{\mathrm{d}t^2} = \frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = \mathbf{F}_i = \sum_{i\neq j}(\mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R)$$
$$\frac{\mathrm{d}C_i}{\mathrm{d}t} = Q_i = \sum_{i\neq j}(Q_{ij}^D + Q_{ij}^R) + Q_i^S$$

where the three components of F_i including the conservative force F_{ij}^C, dissipative force F_{ij}^C and random force F_{ij}^C are expressed as

$$\begin{aligned}
\mathbf{F}_{ij}^C &= A\omega_C(r_{ij})\mathbf{e}_{ij} \\
\mathbf{F}_{ij}^D &= -\gamma\omega_D(r_{ij})(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})\mathbf{e}_{ij} \\
\mathbf{F}_{ij}^R &= \sigma\omega_R(r_{ij})\xi_{ij}\Delta t^{-1/2}\mathbf{e}_{ij} \\
\omega_C(r) &= 1 - r/r_c \\
\omega_D(r) &= \omega_R^2(r) = (1 - r/r_c)^{\mathrm{power_f}} \\
\sigma^2 &= 2\gamma k_B T
\end{aligned}$$

The concentration flux between two tDPD particles includes the Fickian flux Q_{ij}^D and random flux Q_{ij}^R, which are given by

$$\begin{aligned}
Q_{ij}^D &= -\kappa_{ij} w_{DC}(r_{ij})\,(C_i - C_j) \\
Q_{ij}^R &= \epsilon_{ij}\,(C_i + C_j)\,w_{RC}(r_{ij})\xi_{ij} \\
w_{DC}(r_{ij}) &= w_{RC}^2(r_{ij}) = (1 - r/r_{cc})^{\mathrm{power_cc}} \\
\epsilon_{ij}^2 &= m_s^2\kappa_{ij}\rho
\end{aligned}$$

where the parameters kappa and epsilon determine the strength of the Fickian and random fluxes. m_s is the mass of a single solute molecule. In general, m_s is much smaller than the mass of a tDPD particle *m*. For more details, see *(Li2015_JCP)*.

The following coefficients must be defined for each pair of atom types via the *pair_coeff* command as in the examples above.

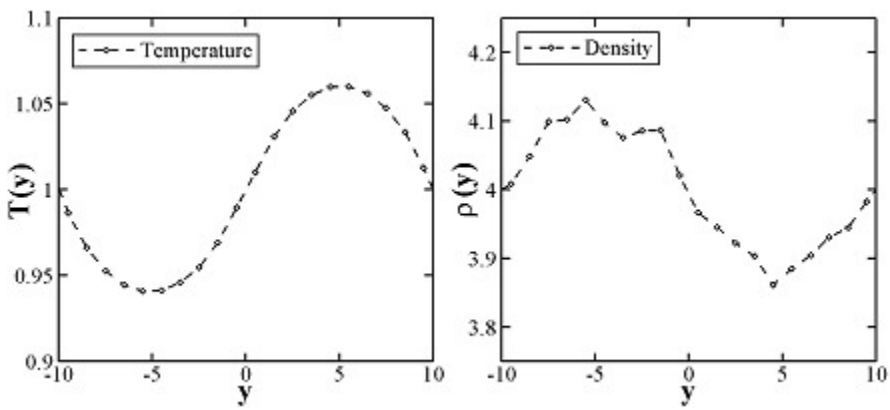
- A (force units)
- γ (force/velocity units)
- power_f (positive real)

- cutoff (distance units)
- cutoff_CC (distance units)
- κ_i (diffusivity units)
- ϵ_i (diffusivity units)
- power_cc_i (positive real)

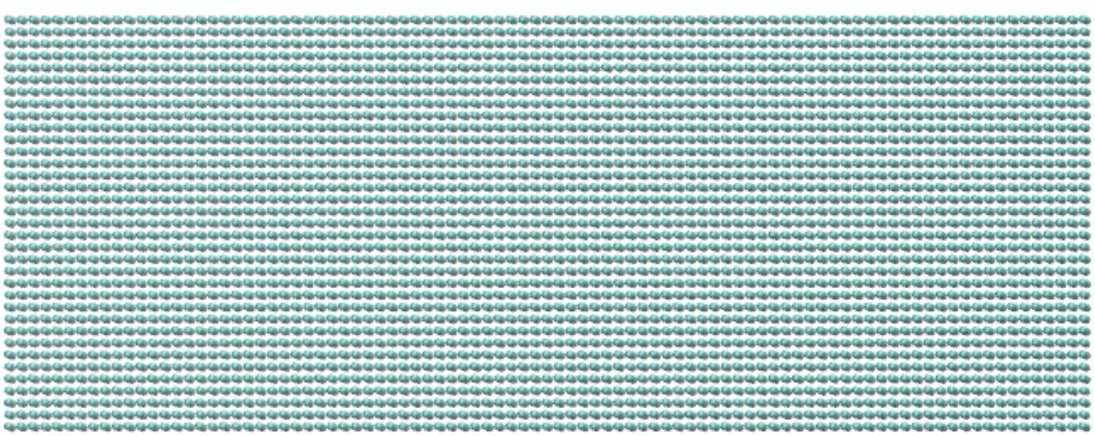
The last 3 values must be repeated Nspecies times, so that values for each of the Nspecies chemical species are specified, as indicated by the "I" suffix. In the first pair_coeff example above for pair_style tdpd, Nspecies = 1. In the second example, Nspecies = 2, so 3 additional coeffs are specified (for species 2).

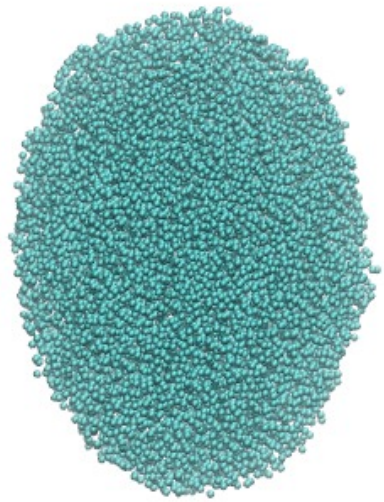
Example scripts

There are example scripts for using all these pair styles in examples/USER/meso. The example for an eDPD simulation models heat conduction with source terms analog of periodic Poiseuille flow problem. The setup follows Fig.12 in *(Li2014_JCP)*. The output of the short eDPD simulation (about 2 minutes on a single core) gives a temperature and density profiles as



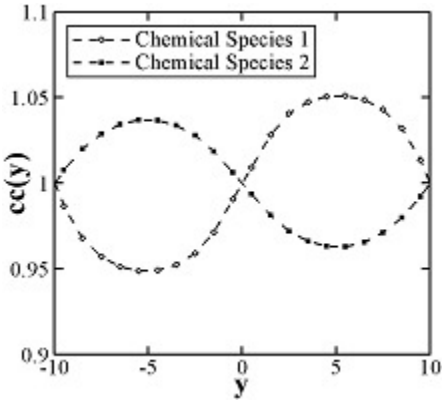
The example for a mDPD simulation models the oscillations of a liquid droplet started from a liquid film. The mDPD parameters are adopted from *(Li2013_POF)*. The short mDPD run (about 2 minutes on a single core) generates a particle trajectory which can be visualized as follows.





The first image is the initial state of the simulation. If you click it a GIF movie should play in your browser. The second image is the final state of the simulation.

The example for a tDPD simulation computes the effective diffusion coefficient of a tDPD system using a method analogous to the periodic Poiseuille flow. The tDPD system is specified with two chemical species, and the setup follows Fig.1 in *(Li2015_JCP)*. The output of the short tDPD simulation (about one and a half minutes on a single core) gives the concentration profiles of the two chemical species as



Mixing, shift, table, tail correction, restart, rRESPA info:

The styles *edpd*, *mdpd*, *mdpd/rhosum* and *tdpd* do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

The styles *edpd*, *mdpd*, *mdpd/rhosum* and *tdpd* do not support the *pair_modify* shift, table, and tail options.

The styles *edpd*, *mdpd*, *mdpd/rhosum* and *tdpd* do not write information to *binary restart files*. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

18.324.4 Restrictions

The pair styles *edpd*, *mdpd*, *mdpd/rhosum* and *tdpd* are part of the USER-MESO package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.324.5 Related commands

pair_coeff, *fix mvv/dpd*, *fix mvv/edpd*, *fix mvv/tdpd*, *fix edpd/source*, *fix tdpd/source*, *compute edpd/temp/atom*, *compute tdpd/cc/atom*

Default: none

(Li2014_JCP) Li, Tang, Lei, Caswell, Karniadakis, J Comput Phys, 265: 113-127 (2014). DOI: 10.1016/j.jcp.2014.02.003.

(Li2015_CC) Li, Tang, Li, Karniadakis, Chem Commun, 51: 11038-11040 (2015). DOI: 10.1039/C5CC01684C.

(Li2013_POF) Li, Hu, Wang, Ma, Zhou, Phys Fluids, 25: 072103 (2013). DOI: 10.1063/1.4812366.

(Li2015_JCP) Li, Yazdani, Tartakovsky, Karniadakis, J Chem Phys, 143: 014101 (2015). DOI: 10.1063/1.4923254.

18.325 pair_style mesocnt command

18.325.1 Syntax

```
pair_style mesocnt
```

18.325.2 Examples

```
pair_style mesocnt
pair_coeff * * 10_10.cnt
```

18.325.3 Description

Style *mesocnt* implements a mesoscopic potential for the interaction of carbon nanotubes (CNTs). In this potential, CNTs are modelled as chains of cylindrical segments in which each infinitesimal surface element interacts with all other CNT surface elements with the Lennard-Jones (LJ) term adopted from the *airebo* style. The interaction energy is then computed by integrating over the surfaces of all interacting CNTs.

The potential is based on interactions between one cylindrical segment and infinitely or semi-infinitely long CNTs as described in *(Volkov1)*. Chains of segments are converted to these (semi-)infinite CNTs bases on an approximate chain approach outlined in *(Volkov2)*. This allows to simplify the computation of the interactions significantly and reduces the computational times to the same order of magnitude as for regular bead spring models where beads interact with the standard *pair_lj/cut* potential.

In LAMMPS, cylindrical segments are represented by bonds. Each segment is defined by its two end points ("nodes") which correspond to atoms in LAMMPS. For the exact functional form of the potential and implementation details, the reader is referred to the original papers *(Volkov1)* and *(Volkov2)*.

The potential requires tabulated data provided in a single ASCII text file specified in the *pair_coeff* command. The first line of the file provides a time stamp and general information. The second line lists four integers giving the number

of data points provided in the subsequent four data tables. The third line lists four floating point numbers: the CNT radius R, the LJ parameter sigma and two numerical parameters delta1 and delta2. These four parameters are given in Angstroms. This is followed by four data tables each separated by a single empty line. The first two tables have two columns and list the parameters uInfParallel and Gamma respectively. The last two tables have three columns giving data on a quadratic array and list the parameters Phi and uSemiParallel respectively. uInfParallel and uSemiParallel are given in eV/Angstrom, Phi is given in eV and Gamma is unitless.

Potential files for CNTs can be readily generated using the freely available code provided on

```
https://github.com/phankl/cntpot
```

Using the same approach, it should also be possible to generate potential files for other 1D systems such as boron nitride nanotubes.

Note: LAMMPS comes with one *mesocnt* style potential file where the default number of data points per table is 1001. This is sufficient for NVT simulations. For proper energy conservation, we recommend using a potential file where the resolution for Phi is at least 2001 data points.

Note: The *mesocnt* style requires CNTs to be represented as a chain of atoms connected by bonds. Atoms need to be numbered consecutively within one chain. Atoms belonging to different CNTs need to be assigned different molecule IDs.

A full summary of the method and LAMMPS implementation details is expected to soon become available in Computer Physics Communications.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support mixing.

This pair style does not support the *pair_modify* shift, table, and tail options.

The *mesocnt* pair style do not write their information to *binary restart files*, since it is stored in tabulated potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

18.325.4 Restrictions

This style is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This pair potential requires the *newton* setting to be "on" for pair interactions.

18.325.5 Related commands

pair_coeff

Default: none

(Volkov1) Volkov and Zhigilei, J Phys Chem C, 114, 5513 (2010).

(Volkov2) Volkov, Simov and Zhigilei, APS Meeting Abstracts, Q31.013 (2008).

18.326 pair_style mgpt command

18.326.1 Syntax

```
pair_style mgpt
```

18.326.2 Examples

```
pair_style mgpt
pair_coeff * * Ta6.8x.mgpt.parmin Ta6.8x.mgpt.potin Omega
cp ~/lammps/potentials/Ta6.8x.mgpt.parmin parmin
cp ~/lammps/potentials/Ta6.8x.mgpt.potin potin
pair_coeff * * parmin potin Omega volpress yes nbody 1234 precision double
pair_coeff * * parmin potin Omega volpress yes nbody 12
```

18.326.3 Description

Within DFT quantum mechanics, generalized pseudopotential theory (GPT) (*Moriarty1*) provides a first-principles approach to multi-ion interatomic potentials in d-band transition metals, with a volume-dependent, real-space total-energy functional for the N-ion elemental bulk material in the form

$$E_{\rm tot}(\mathbf{R}_1 \ldots \mathbf{R}_N) = NE_{\rm vol}(\Omega) + \frac{1}{2}\sum_{i,j}{}' \, v_2(ij;\Omega) + \frac{1}{6}\sum_{i,j,k}{}' \, v_3(ijk;\Omega) + \frac{1}{24}\sum_{i,j,k,l}{}' \, v_4(ijkl;\Omega)$$

where the prime on each summation sign indicates the exclusion of all self-interaction terms from the summation. The leading volume term E_vol as well as the two-ion central-force pair potential v_2 and the three- and four-ion angular-force potentials, v_3 and v_4, depend explicitly on the atomic volume Omega, but are structure independent and transferable to all bulk ion configurations, either ordered or disordered, and with of without the presence of point and line defects. The simplified model GPT or MGPT (*Moriarty2*, *Moriarty3*), which retains the form of E_tot and permits more efficient large-scale atomistic simulations, derives from the GPT through a series of systematic approximations applied to E_vol and the potentials v_n that are valid for mid-period transition metals with nearly half-filled d bands.

Both analytic (*Moriarty2*) and matrix (*Moriarty3*) representations of MGPT have been developed. In the more general matrix representation, which can also be applied to f-band actinide metals and permits both canonical and non-canonical d/f bands, the multi-ion potentials are evaluated on the fly during a simulation through d- or f-state matrix multiplication, and the forces that move the ions are determined analytically. Fast matrix-MGPT algorithms have been developed independently by Glosli (*Glosli*, *Moriarty3*) and by Oppelstrup (*Oppelstrup*)

The *mgpt* pair style calculates forces, energies, and the total energy per atom, E_tot/N, using the Oppelstrup matrix-MGPT algorithm. Input potential and control data are entered through the *pair_coeff* command. Each material treated

requires input parmin and potin potential files, as shown in the above examples, as well as specification by the user of the initial atomic volume Omega through pair_coeff. At the beginning of a time step in any simulation, the total volume of the simulation cell V should always be equal to Omega*N, where N is the number of metal ions present, taking into account the presence of any vacancies and/or interstitials in the case of a solid. In a constant-volume simulation, which is the normal mode of operation for the *mgpt* pair style, Omega, V and N all remain constant throughout the simulation and thus are equal to their initial values. In a constant-stress simulation, the cell volume V will change (slowly) as the simulation proceeds. After each time step, the atomic volume should be updated by the code as Omega = V/N. In addition, the volume term E_vol and the potentials v_2, v_3 and v_4 have to be removed at the end of the time step, and then respecified at the new value of Omega. In all simulations, Omega must remain within the defined volume range for E_vol and the potentials for the given material.

The default option volpress yes in the *pair_coeff* command includes all volume derivatives of E_tot required to calculate the stress tensor and pressure correctly. The option volpress no disregards the pressure contribution resulting from the volume term E_vol, and can be used for testing and analysis purposes. The additional optional variable nbody controls the specific terms in E_tot that are calculated. The default option and the normal option for mid-period transition and actinide metals is nbody 1234 for which all four terms in E_tot are retained. The option nbody 12, for example, retains only the volume term and the two-ion pair potential term and can be used for GPT series-end transition metals that can be well described without v_3 and v_4. The nbody option can also be used to test or analyze the contribution of any of the four terms in E_tot to a given calculated property.

The *mgpt* pair style makes extensive use of matrix algebra and includes optimized kernels for the BlueGene/Q architecture and the Intel/AMD (x86) architectures. When compiled with the appropriate compiler and compiler switches (-msse3 on x86, and using the IBM XL compiler on BG/Q), these optimized routines are used automatically. For BG/Q machines, building with the default Makefile for that architecture (e.g., "make bgq") should enable the optimized algebra routines. For x-86 machines, there is a provided Makefile.mgptfast which enables the fast algebra routines, i.e. build LAMMPS with "make mgptfast". The user will be informed in the output files of the matrix kernels in use. To further improve speed, on x86 the option precision single can be added to the *pair_coeff* command line, which improves speed (up to a factor of two) at the cost of doing matrix calculations with 7 digit precision instead of the default 16. For consistency the default option can be specified explicitly by the option precision double.

All remaining potential and control data are contained with the parmin and potin files, including cutoffs, atomic mass, and other basic MGPT variables. Specific MGPT potential data for the transition metals tantalum (Ta4 and Ta6.8x potentials), molybdenum (Mo5.2 potentials), and vanadium (V6.1 potentials) are contained in the LAMMPS potentials directory. The stored files are, respectively, Ta4.mgpt.parmin, Ta4.mgpt.potin, Ta6.8x.mgpt.parmin, Ta6.8x.mgpt.potin, Mo5.2.mgpt.parmin, Mo5.2.mgpt.potin, V6.1.mgpt.parmin, and V6.1.mgpt.potin . Useful corresponding informational "README" files on the Ta4, Ta6.8x, Mo5.2 and V6.1 potentials are also included in the potentials directory. These latter files indicate the volume mesh and range for each potential and give appropriate references for the potentials. It is expected that MGPT potentials for additional materials will be added over time.

Useful example MGPT scripts are given in the examples/USER/mgpt directory. These scripts show the necessary steps to perform constant-volume calculations and simulations. It is strongly recommended that the user work through and understand these examples before proceeding to more complex simulations.

Note: For good performance, LAMMPS should be built with the compiler flags "-O3 -msse3 -funroll-loops" when including this pair style. The src/MAKE/OPTIONS/Makefile.mgptfast is an example machine Makefile with these options included as part of a standard MPI build. Note that it as provided, it will build with whatever low-level compiler (g++, icc, etc) is the default for your MPI installation.

Mixing, shift, table tail correction, restart:

This pair style does not support the *pair_modify* mix, shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in potential files. Thus, you needs to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.326.4 Restrictions

This pair style is part of the USER-MGPT package and is only enabled if LAMMPS is built with that package. See the *Build package* doc page for more info.

The MGPT potentials require the *newton* setting to be "on" for pair style interactions.

The stored parmin and potin potential files provided with LAMMPS in the "potentials" directory are written in Rydberg atomic units, with energies in Rydbergs and distances in Bohr radii. The *mgpt* pair style converts Rydbergs to Hartrees to make the potential files compatible with LAMMPS electron *units*.

The form of E_tot used in the *mgpt* pair style is only appropriate for elemental bulk solids and liquids. This includes solids with point and extended defects such as vacancies, interstitials, grain boundaries and dislocations. Alloys and free surfaces, however, require significant modifications, which are not included in the *mgpt* pair style. Likewise, the *hybrid* pair style is not allowed, where MGPT would be used for some atoms but not for others.

Electron-thermal effects are not included in the standard MGPT potentials provided in the "potentials" directory, where the potentials have been constructed at zero electron temperature. Physically, electron-thermal effects may be important in 3d (e.g., V) and 4d (e.g., Mo) transition metals at high temperatures near melt and above. It is expected that temperature-dependent MGPT potentials for such cases will be added over time.

18.326.5 Related commands

pair_coeff

18.326.6 Default

The options defaults for the *pair_coeff* command are volpress yes, nbody 1234, and precision double.

(Moriarty1) Moriarty, Physical Review B, 38, 3199 (1988).

(Moriarty2) Moriarty, Physical Review B, 42, 1609 (1990). Moriarty, Physical Review B 49, 12431 (1994).

(Moriarty3) Moriarty, Benedict, Glosli, Hood, Orlikowski, Patel, Soderlind, Streitz, Tang, and Yang, Journal of Materials Research, 21, 563 (2006).

(Glosli) Glosli, unpublished, 2005. Streitz, Glosli, Patel, Chan, Yates, de Supinski, Sexton and Gunnels, Journal of Physics: Conference Series, 46, 254 (2006).

(Oppelstrup) Oppelstrup, unpublished, 2015. Oppelstrup and Moriarty, to be published.

18.327 pair_style mie/cut command

18.328 pair_style mie/cut/gpu command

18.328.1 Syntax

```
pair_style mie/cut cutoff
```

- cutoff = global cutoff for mie/cut interactions (distance units)

18.328.2 Examples

```
pair_style mie/cut 10.0
pair_coeff 1 1 0.72 3.40 23.00 6.66
pair_coeff 2 2 0.30 3.55 12.65 6.00
pair_coeff 1 2 0.46 3.32 16.90 6.31
```

18.328.3 Description

The *mie/cut* style computes the Mie potential, given by

$$E = C\epsilon \left[\left(\frac{\sigma}{r}\right)^{\gamma_{rep}} - \left(\frac{\sigma}{r}\right)^{\gamma_{att}} \right] \qquad r < r_c$$

Rc is the cutoff and C is a function that depends on the repulsive and attractive exponents, given by:

$$C = \left(\frac{\gamma_{rep}}{\gamma_{rep} - \gamma_{att}}\right) \left(\frac{\gamma_{rep}}{\gamma_{att}}\right)^{\left(\frac{\gamma_{att}}{\gamma_{rep} - \gamma_{att}}\right)}$$

Note that for 12/6 exponents, C is equal to 4 and the formula is the same as the standard Lennard-Jones potential.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- gammaR
- gammaA
- cutoff (distance units)

The last coefficient is optional. If not specified, the global cutoff specified in the pair_style command is used.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the mie/cut pair styles can be mixed. If not explicitly defined, both the repulsive and attractive gamma exponents for different atoms will be calculated following the same mixing rule defined for distances. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style supports the *pair_modify* shift option for the energy of the pair interaction.

This pair style supports the *pair_modify* tail option for adding a long-range tail correction to the energy and pressure of the pair interaction.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style supports the use of the *inner*, *middle*, and *outer* keywords of the *run_style respa* command, meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. See the *run_style* command for details.

18.328.4 Restrictions

none

18.328.5 Related commands

pair_coeff

Default: none

(Mie) G. Mie, Ann Phys, 316, 657 (1903).

(Avendano) C. Avendano, T. Lafitte, A. Galindo, C. S. Adjiman, G. Jackson, E. Muller, J Phys Chem B, 115, 11154 (2011).

18.329 pair_style mm3/switch3/coulgauss/long command

18.329.1 Syntax

```
pair_style style args
```

- style = *mm3/switch3/coulgauss/long*
- args = list of arguments for a particular style

```
mm3/switch3/coulgauss/long args = cutoff (cutoff2) width
  cutoff  = global cutoff for MM3 (and Coulombic if only 1 arg) (distance␣
↪units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
  width  = width parameter of the smoothing function (distance units)
```

18.329.2 Examples

```
pair_style mm3/switch3/coulgauss/long    12.0 3.0
pair_coeff 1  0.2 2.5 1.2

pair_style mm3/switch3/coulgauss/long   12.0 10.0 3.0
pair_coeff 1  0.2 2.5 1.2
```

18.329.3 Description

The *mm3/switch3/coulgauss/long* style evaluates the MM3 vdW potential *(Allinger)*

$$E = \epsilon_{ij} \left[-2.25 \left(\frac{r_{v,ij}}{r_{ij}} \right)^6 + 1.84(10)^5 \exp\left[-12.0 r_{ij}/r_{v,ij} \right] \right] S_3(r_{ij})$$

$$r_{v,ij} = r_{v,i} + r_{v,j}$$

$$\epsilon_{ij} = \sqrt{\epsilon_i \epsilon_j}$$

, which goes smoothly to zero at the cutoff r_c as defined by the switching function

$$S_3(r) = \begin{cases} 1 & \text{if} \quad r < r_\mathrm{c} - w \\ 3x^2 - 2x^3 & \text{if} \quad r < r_\mathrm{c} \quad \text{with} \quad x = \frac{r_\mathrm{c} - r}{w} \\ 0 & \text{if} \quad r >= r_\mathrm{c} \end{cases}$$

where w is the width defined in the arguments. This potential is combined with Coulomb interaction between Gaussian charge densities:

$$E = \frac{q_i q_j \mathrm{erf}\left(r/\sqrt{\gamma_1^2 + \gamma_2^2} \right)}{\epsilon r_{ij}}$$

where q_i and q_j are the charges on the 2 atoms, epsilon is the dielectric constant which can be set by the *dielectric* command, :γ_i and γ_j are the widths of the Gaussian charge distribution and erf() is the error-function. This style has to be used in conjunction with the *kspace_style* command

If one cutoff is specified it is used for both the vdW and Coulomb terms. If two cutoffs are specified, the first is used as the cutoff for the vdW terms, and the second is the cutoff for the Coulombic term.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- ϵ (energy)
- r_v (distance)
- γ (distance)

Mixing, shift, table, tail correction, restart, rRESPA info:

Mixing rules are fixed for this style as defined above.

Shifting the potential energy is not necessary because the switching function ensures that the potential is zero at the cut-off.

18.329.4 Restrictions

These styles are part of the USER-YAFF package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.329.5 Related commands

pair_coeff

Default: none

18.330 pair_style momb command

18.330.1 Syntax

```
pair_style momb cutoff s6 d
```

- cutoff = global cutoff (distance units)
- s6 = global scaling factor of the exchange-correlation functional used (unitless)
- d = damping scaling factor of Grimme's method (unitless)

18.330.2 Examples

```
pair_style momb 12.0 0.75 20.0
pair_style hybrid/overlay eam/fs lj/charmm/coul/long 10.0 12.0 momb 12.0 0.75 20.0␣
↪morse 5.5

pair_coeff 1 2 momb 0.0 1.0 1.0 10.2847 2.361
```

18.330.3 Description

Style *momb* computes pairwise van der Waals (vdW) and short-range interactions using the Morse potential and *(Grimme)* method implemented in the Many-Body Metal-Organic (MOMB) force field described comprehensively in *(Fichthorn)* and *(Zhou)*. Grimme's method is widely used to correct for dispersion in density functional theory calculations.

$$E = D_0[\exp^{-2\alpha(r-r_0)} - 2\exp^{-\alpha(r-r_0)}] - s_6 \frac{C_6}{r^6} f_{damp}(r, R_r)$$

$$f_{damp}(r, R_r) = \frac{1}{1 + \exp^{-d(r/R_r - 1)}}$$

For the *momb* pair style, the following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* as described below:

- D_0 (energy units)
- α (1/distance units)
- r_0 (distance units)
- C_6 (energy*distance^6 units)

- R_r (distance units, typically sum of atomic vdW radii)

18.330.4 Restrictions

This style is part of the USER-MISC package. It is only enabled if LAMMPS is built with that package. See the *Build package* doc page on for more info.

18.330.5 Related commands

pair_coeff, *pair_style morse*

Default: none

(Grimme) Grimme, J Comput Chem, 27(15), 1787-1799 (2006).

(Fichthorn) Fichthorn, Balankura, Qi, CrystEngComm, 18(29), 5410-5417 (2016).

(Zhou) Zhou, Saidi, Fichthorn, J Phys Chem C, 118(6), 3366-3374 (2014).

18.331 pair_style morse command

18.332 pair_style morse/gpu command

18.333 pair_style morse/omp command

18.334 pair_style morse/opt command

18.335 pair_style morse/smooth/linear command

18.336 pair_style morse/smooth/linear/omp command

18.337 pair_style morse/kk command

18.337.1 Syntax

```
pair_style style args
```

- style = *morse* or *morse/smooth/linear* or *morse/soft*
- args = list of arguments for a particular style

```
morse args = cutoff
  cutoff = global cutoff for Morse interactions (distance units)
morse/smooth/linear args = cutoff
  cutoff = global cutoff for Morse interactions (distance units)
```

18.337.2 Examples

```
pair_style morse 2.5
pair_style morse/smooth/linear 2.5
pair_coeff * * 100.0 2.0 1.5
pair_coeff 1 1 100.0 2.0 1.5 3.0
```

18.337.3 Description

Style *morse* computes pairwise interactions with the formula

$$E = D_0 \left[e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)} \right] \qquad r < r_c$$

Rc is the cutoff.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- D_0 (energy units)
- α (1/distance units)
- r_0 (distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global morse cutoff is used.

The *morse/smooth/linear* variant is similar to the lj/smooth/linear variant in that it adds to the potential a shift and a linear term so that both, potential energy and force, go to zero at the cut-off:

$$\phi(r) = D_0 \left[e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)} \right] \qquad r < r_c$$

$$E(r) = \phi(r) - \phi(R_c) - (r - R_c) \left. \frac{d\phi}{dr} \right|_{r=R_c} \qquad r < R_c$$

The syntax of the pair_style and pair_coeff commands are the same for the *morse* and *morse/smooth/linear* styles.

A version of the *morse* style with a soft core, *morse/soft*, suitable for use in free energy calculations, is part of the USER-FEP package and is documented with the *pair_style */soft* styles. The version with soft core is only available if LAMMPS was built with that package. See the *Build package* doc page for more info.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

None of these pair styles support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

All of these pair styles support the *pair_modify* shift option for the energy of the pair interaction.

The *pair_modify* table options is not relevant for the Morse pair styles.

None of these pair styles support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

All of these pair styles write their information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

18.337.4 Restrictions

The *morse/smooth/linear* pair style is only enabled if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

18.337.5 Related commands

pair_coeff, *pair_style */soft*

Default: none

18.338 pair_style multi/lucy command

18.338.1 Syntax

```
pair_style multi/lucy style N keyword ...
```

- style = *lookup* or *linear* = method of interpolation
- N = use N values in *lookup*, *linear* tables

18.338.2 Examples

```
pair_style multi/lucy linear 1000
pair_coeff * * multibody.table ENTRY1 7.0
```

18.338.3 Description

Style *multi/lucy* computes a density-dependent force following from the many-body form described in *(Moore)* and *(Warren)* as

$$F_i^{DD}(\rho_i, \rho_j, r_{ij}) = \frac{1}{2}\omega_{DD}\left(r_{ij}\right)\left[A\left(\rho_i\right) + A\left(\rho_j\right)\right]e_{ij}$$

which consists of a density-dependent function, $A(\rho)$, and a radial-dependent weight function, $\omega_{DD}(r_{ij})$. The radial-dependent weight function, $\omega_{DD}(r_{ij})$, is taken as the Lucy function:

$$\omega_{DD}\left(r_{ij}\right) = \left(1 + \frac{3r_{ij}}{r_{cut}}\right)\left(1 + \frac{r_{ij}}{r_{cut}}\right)^3$$

The density-dependent energy for a given particle is given by:

$$u_i^{DD}\left(\rho_i\right) = \frac{\pi r_{cut}^4}{84}\int_{\rho_0}^{\rho_i} A\left(\rho'\right)d\rho'$$

See the supporting information of *(Brennan)* or the publication by *(Moore)* for more details on the functional form.

An interpolation table is used to evaluate the density-dependent energy ($\int A(\rho')d\rho'$) and force ($A(\rho')$). Note that the pre-factor to the energy is computed after the interpolation, thus the $\int A(\rho')d\rho'$ will have units of energy / length^4.

The interpolation table is created as a pre-computation by fitting cubic splines to the file values and interpolating the density-dependent energy and force at each of *N* densities. During a simulation, the tables are used to interpolate the density-dependent energy and force as needed for each pair of particles separated by a distance *R*. The interpolation is done in one of 2 styles: *lookup* and *linear*.

For the *lookup* style, the density is used to find the nearest table entry, which is the density-dependent energy and force.

For the *linear* style, the density is used to find the 2 surrounding table values from which the density-dependent energy and force are computed by linear interpolation.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above.

- filename
- keyword
- cutoff (distance units)

The filename specifies a file containing the tabulated density-dependent energy and force. The keyword specifies a section of the file. The cutoff is an optional coefficient. If not specified, the outer cutoff in the table itself (see below) will be used to build an interpolation table that extend to the largest tabulated distance. If specified, only file values up to the cutoff are used to create the interpolation table. The format of this file is described below.

The format of a tabulated file is a series of one or more sections, defined as follows (without the parenthesized comments):

```
# Density-dependent function (one or more comment or blank lines)

DD-FUNCTION                 (keyword is first text on line)
N 500 R 1.0 10.0            (N, R, RSQ parameters)
                            (blank)
1 1.0 25.5 102.34           (index, density, energy/r^4, force)
2 1.02 23.4 98.5
...
500 10.0 0.001 0.003
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the pair_coeff command. The next line lists (in any order) one or more parameters for the table. Each parameter is a keyword followed by one or more numeric values.

The parameter "N" is required and its value is the number of table entries that follow. Note that this may be different than the *N* specified in the *pair_style multi/lucy* command. Let Ntable = *N* in the pair_style command, and Nfile = "N" in the tabulated file. What LAMMPS does is a preliminary interpolation by creating splines using the Nfile tabulated values as nodal points. It uses these to interpolate the density-dependent energy and force at Ntable different points. The resulting tables of length Ntable are then used as described above, when computing the density-dependent energy and force. This means that if you want the interpolation tables of length Ntable to match exactly what is in the tabulated file (with effectively no preliminary interpolation), you should set Ntable = Nfile, and use the "RSQ" parameter. This is because the internal table abscissa is always RSQ (separation distance squared), for efficient lookup.

All other parameters are optional. If "R" or "RSQ" does not appear, then the distances in each line of the table are used as-is to perform spline interpolation. In this case, the table values can be spaced in *density* uniformly or however you wish to position table values in regions of large gradients.

If used, the parameters "R" or "RSQ" are followed by 2 values *rlo* and *rhi*. If specified, the density associated with each density-dependent energy and force value is computed from these 2 values (at high accuracy), rather than using the (low-accuracy) value listed in each line of the table. The density values in the table file are ignored in this case. For "R", distances uniformly spaced between *rlo* and *rhi* are computed; for "RSQ", squared distances uniformly spaced between *rlo**rlo* and *rhi**rhi* are computed.

Note: If you use "R" or "RSQ", the tabulated distance values in the file are effectively ignored, and replaced by new values as described in the previous paragraph. If the density value in the table is not very close to the new value (i.e. round-off difference), then you will be assigning density-dependent energy and force values to a different density, which is probably not what you want. LAMMPS will warn if this is occurring.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is r (in density units), the 3rd value is the density-dependent function value (in energy units / length^4), and the 4th is the force (in force units). The density values must increase from one line to the next.

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

The *pair_modify* shift, table, and tail options are not relevant for this pair style.

This pair style writes the settings for the "pair_style multi/lucy" command to *binary restart files*, so a pair_style command does not need to specified in an input script that reads a restart file. However, the coefficient information is not stored in the restart file, since it is tabulated in the potential files. Thus, pair_coeff commands do need to be specified in the restart input script.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.338.4 Restrictions

This command is part of the USER-DPD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.338.5 Related commands

pair_coeff

Default: none

(Warren) Warren, Phys Rev E, 68, 066702 (2003).

(Brennan) Brennan, J Chem Phys Lett, 5, 2144-2149 (2014).

(Moore) Moore, J Chem Phys, 144, 104501 (2016).

18.339 pair_style multi/lucy/rx command

18.340 pair_style multi/lucy/rx/kk command

18.340.1 Syntax

```
pair_style multi/lucy/rx style N keyword ...
```

- style = *lookup* or *linear* = method of interpolation
- N = use N values in *lookup*, *linear* tables
- weighting = fractional or molecular (optional)

18.340.2 Examples

```
pair_style multi/lucy/rx linear 1000
pair_style multi/lucy/rx linear 1000 fractional
pair_style multi/lucy/rx linear 1000 molecular
pair_coeff * * multibody.table ENTRY1 h2o h2o 7.0
pair_coeff * * multibody.table ENTRY1 h2o 1fluid 7.0
```

18.340.3 Description

Style *multi/lucy/rx* is used in reaction DPD simulations, where the coarse-grained (CG) particles are composed of *m* species whose reaction rate kinetics are determined from a set of *n* reaction rate equations through the *fix rx* command. The species of one CG particle can interact with a species in a neighboring CG particle through a site-site interaction potential model. Style *multi/lucy/rx* computes the site-site density-dependent force following from the many-body form described in *(Moore)* and *(Warren)* as

$$F_i^{DD}(\rho_i, \rho_j, r_{ij}) = \frac{1}{2}\omega_{DD}(r_{ij})\left[A(\rho_i) + A(\rho_j)\right]e_{ij}$$

which consists of a density-dependent function, $A(\rho)$, and a radial-dependent weight function, $\omega_{DD}(r_{ij})$. The radial-dependent weight function, $\omega_{DD}(r_{ij})$, is taken as the Lucy function:

$$\omega_{DD}\left(r_{ij}\right) = \left(1 + \frac{3r_{ij}}{r_{cut}}\right)\left(1 + \frac{r_{ij}}{r_{cut}}\right)^3$$

The density-dependent energy for a given particle is given by:

$$u_i^{DD}\left(\rho_i\right) = \frac{\pi r_{cut}^4}{84}\int_{\rho_0}^{\rho_i} A\left(\rho'\right) d\rho'$$

See the supporting information of *(Brennan)* or the publication by *(Moore)* for more details on the functional form.

An interpolation table is used to evaluate the density-dependent energy ($\int A(\rho')d\rho'$) and force ($A(\rho')$). Note that the pre-factor to the energy is computed after the interpolation, thus the $\int A(\rho')d\rho'$ will have units of energy / length^4.

The interpolation table is created as a pre-computation by fitting cubic splines to the file values and interpolating the density-dependent energy and force at each of *N* densities. During a simulation, the tables are used to interpolate the density-dependent energy and force as needed for each pair of particles separated by a distance *R*. The interpolation is done in one of 2 styles: *lookup* and *linear*.

For the *lookup* style, the density is used to find the nearest table entry, which is the density-dependent energy and force.

For the *linear* style, the density is used to find the 2 surrounding table values from which the density-dependent energy and force are computed by linear interpolation.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above.

- filename
- keyword
- species1
- species2
- cutoff (distance units)

The filename specifies a file containing the tabulated density-dependent energy and force. The keyword specifies a section of the file. The cutoff is an optional coefficient. If not specified, the outer cutoff in the table itself (see below) will be used to build an interpolation table that extend to the largest tabulated distance. If specified, only file values up to the cutoff are used to create the interpolation table. The format of this file is described below.

The species tags define the site-site interaction potential between two species contained within two different particles. The species tags must either correspond to the species defined in the reaction kinetics files specified with the *fix rx* command or they must correspond to the tag "1fluid", signifying interaction with a product species mixture determined through a one-fluid approximation. The interaction potential is weighted by the geometric average of either the mole fraction concentrations or the number of molecules associated with the interacting coarse-grained particles (see the *fractional* or *molecular* weighting pair style options). The coarse-grained potential is stored before and after the reaction kinetics solver is applied, where the difference is defined to be the internal chemical energy (uChem).

The format of a tabulated file is a series of one or more sections, defined as follows (without the parenthesized comments):

```
# Density-dependent function (one or more comment or blank lines)

DD-FUNCTION                (keyword is first text on line)
N 500 R 1.0 10.0           (N, R, RSQ parameters)
```

```
                              (blank)
1 1.0 25.5 102.34             (index, density, energy/r^4, force)
2 1.02 23.4 98.5
...
500 10.0 0.001 0.003
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the pair_coeff command. The next line lists (in any order) one or more parameters for the table. Each parameter is a keyword followed by one or more numeric values.

The parameter "N" is required and its value is the number of table entries that follow. Note that this may be different than the *N* specified in the *pair_style multi/lucy/rx* command. Let Ntable = *N* in the pair_style command, and Nfile = "N" in the tabulated file. What LAMMPS does is a preliminary interpolation by creating splines using the Nfile tabulated values as nodal points. It uses these to interpolate the density-dependent energy and force at Ntable different points. The resulting tables of length Ntable are then used as described above, when computing the density-dependent energy and force. This means that if you want the interpolation tables of length Ntable to match exactly what is in the tabulated file (with effectively no preliminary interpolation), you should set Ntable = Nfile, and use the "RSQ" parameter. This is because the internal table abscissa is always RSQ (separation distance squared), for efficient lookup.

All other parameters are optional. If "R" or "RSQ" does not appear, then the distances in each line of the table are used as-is to perform spline interpolation. In this case, the table values can be spaced in *density* uniformly or however you wish to position table values in regions of large gradients.

If used, the parameters "R" or "RSQ" are followed by 2 values *rlo* and *rhi*. If specified, the density associated with each density-dependent energy and force value is computed from these 2 values (at high accuracy), rather than using the (low-accuracy) value listed in each line of the table. The density values in the table file are ignored in this case. For "R", distances uniformly spaced between *rlo* and *rhi* are computed; for "RSQ", squared distances uniformly spaced between *rlo**rlo* and *rhi**rhi* are computed.

Note: If you use "R" or "RSQ", the tabulated distance values in the file are effectively ignored, and replaced by new values as described in the previous paragraph. If the density value in the table is not very close to the new value (i.e. round-off difference), then you will be assigning density-dependent energy and force values to a different density, which is probably not what you want. LAMMPS will warn if this is occurring.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is r (in density units), the 3rd value is the density-dependent function value (in energy units / length^4), and the 4th is the force (in force units). The density values must increase from one line to the next.

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

The *pair_modify* shift, table, and tail options are not relevant for this pair style.

This pair style writes the settings for the "pair_style multi/lucy/rx" command to *binary restart files*, so a pair_style command does not need to specified in an input script that reads a restart file. However, the coefficient information is not stored in the restart file, since it is tabulated in the potential files. Thus, pair_coeff commands do need to be specified in the restart input script.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

18.340.4 Restrictions

This command is part of the USER-DPD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.340.5 Related commands

pair_coeff

Default: fractional weighting

(Warren) Warren, Phys Rev E, 68, 066702 (2003).

(Brennan) Brennan, J Chem Phys Lett, 5, 2144-2149 (2014).

(Moore) Moore, J Chem Phys, 144, 104501 (2016).

18.341 pair_style nb3b/harmonic command

18.341.1 Syntax

```
pair_style nb3b/harmonic
```

18.341.2 Examples

```
pair_style nb3b/harmonic
pair_coeff * * MgOH.nb3bharmonic Mg O H
```

18.341.3 Description

This pair style computes a non-bonded 3-body harmonic potential for the energy E of a system of atoms as

$$E = K(\theta - \theta_0)^2$$

where θ_0 is the equilibrium value of the angle and K is a prefactor. Note that the usual 1/2 factor is included in K. The form of the potential is identical to that used in angle_style *harmonic*, but in this case, the atoms do not need to be explicitly bonded.

Only a single pair_coeff command is used with this style which specifies a potential file with parameters for specified elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of elements to atom types

See the *pair_coeff* doc page for alternate ways to specify the path for the potential file.

As an example, imagine a file SiC.nb3b.harmonic has potential values for Si and C. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * SiC.nb3b.harmonic Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the potential file. The final C argument maps LAMMPS atom type 4 to the C element in the potential file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when the potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials. An example of a pair_coeff command for use with the *hybrid* pair style is:

pair_coeff * * nb3b/harmonic MgOH.nb3b.harmonic Mg O H

Three-body non-bonded harmonic files in the *potentials* directory of the LAMMPS distribution have a ".nb3b.harmonic" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements.

Each entry has six arguments. The first three are atom types as referenced in the LAMMPS input file. The first argument specifies the central atom. The fourth argument indicates the K parameter. The fifth argument indicates θ_0. The sixth argument indicates a separation cutoff in Angstroms.

For a given entry, if the second and third arguments are identical, then the entry is for a cutoff for the distance between types 1 and 2 (values for K and θ_0 are irrelevant in this case).

For a given entry, if the first three arguments are all different, then the entry is for the K and θ_0 parameters (the cutoff in this case is irrelevant).

It is required that the potential file contains entries for *all* permutations of the elements listed in the pair_coeff command. If certain combinations are not parameterized the corresponding parameters should be set to zero. The potential file can also contain entries for additional elements which are not used in a particular simulation; LAMMPS ignores those entries.

18.341.4 Restrictions

This pair style can only be used if LAMMPS was built with the MANYBODY package. See the *Build package* doc page for more info.

18.341.5 Related commands

pair_coeff

Default: none

18.342 pair_style nm/cut command

18.343 pair_style nm/cut/coul/cut command

18.344 pair_style nm/cut/coul/long command

18.345 pair_style nm/cut/omp command

18.346 pair_style nm/cut/coul/cut/omp command

18.347 pair_style nm/cut/coul/long/omp command

18.347.1 Syntax

```
pair_style style args
```

- style = *nm/cut* or *nm/cut/coul/cut* or *nm/cut/coul/long*
- args = list of arguments for a particular style

```
nm/cut args = cutoff
  cutoff = global cutoff for Pair interactions (distance units)
nm/cut/coul/cut args = cutoff (cutoff2)
  cutoff = global cutoff for Pair (and Coulombic if only 1 arg) (distance␣
↪units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
nm/cut/coul/long args = cutoff (cutoff2)
  cutoff = global cutoff for Pair (and Coulombic if only 1 arg) (distance␣
↪units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
```

18.347.2 Examples

```
pair_style nm/cut 12.0
pair_coeff * * 0.01 5.4 8.0 7.0
pair_coeff 1 1 0.01 4.4 7.0 6.0

pair_style nm/cut/coul/cut 12.0 15.0
pair_coeff * * 0.01 5.4 8.0 7.0
pair_coeff 1 1 0.01 4.4 7.0 6.0

pair_style nm/cut/coul/long 12.0 15.0
pair_coeff * * 0.01 5.4 8.0 7.0
pair_coeff 1 1 0.01 4.4 7.0 6.0
```

18.347.3 Description

Style *nm* computes site-site interactions based on the N-M potential by *Clarke*, mainly used for ionic liquids. A site can represent a single atom or a united-atom site. The energy of an interaction has the following form:

$$E = \frac{E_0}{(n-m)} \left[m \left(\frac{r_0}{r}\right)^n - n \left(\frac{r_0}{r}\right)^m \right] \qquad r < r_c$$

where r_c is the cutoff.

Style *nm/cut/coul/cut* adds a Coulombic pairwise interaction given by

$$E = \frac{C q_i q_j}{\epsilon r} \qquad r < r_c$$

where C is an energy-conversion constant, q_i and q_j are the charges on the 2 atoms, and epsilon is the dielectric constant which can be set by the *dielectric* command. If one cutoff is specified in the pair_style command, it is used for both the N-M and Coulombic terms. If two cutoffs are specified, they are used as cutoffs for the N-M and Coulombic terms respectively.

Styles *nm/cut/coul/long* compute the same Coulombic interactions as style *nm/cut/coul/cut* except that an additional damping factor is applied to the Coulombic term so it can be used in conjunction with the *kspace_style* command and its *ewald* or *pppm* option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

For all of the *nm* pair styles, the following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands.

- E_0 (energy units)
- r_0 (distance units)
- n (unitless)
- m (unitless)
- cutoff1 (distance units)
- cutoff2 (distance units)

The latter 2 coefficients are optional. If not specified, the global N-M and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both N-M and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the N-M and Coulombic cutoffs for this type pair. You cannot specify 2 cutoffs for style *nm*, since it has no Coulombic terms.

For *nm/cut/coul/long* only the N-M cutoff can be specified since a Coulombic cutoff cannot be specified for an individual I,J type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

All of the *nm* pair styles supports the *pair_modify* shift option for the energy of the pair interaction.

The *nm/cut/coul/long* pair styles support the *pair_modify* table option since they can tabulate the short-range portion of the long-range Coulombic interaction.

All of the *nm* pair styles support the *pair_modify* tail option for adding a long-range tail correction to the energy and pressure for the N-M portion of the pair interaction.

All of the *nm* pair styles write their information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

All of the *nm* pair styles can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

18.347.4 Restrictions

These pair styles are part of the MISC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.347.5 Related commands

pair_coeff

Default: none

(Clarke) Clarke and Smith, J Chem Phys, 84, 2290 (1986).

18.348 pair_style none command

18.348.1 Syntax

```
pair_style none
```

18.348.2 Examples

```
pair_style none
```

18.348.3 Description

Using a pair style of none means pair forces and energies are not computed.

With this choice, the force cutoff is 0.0, which means that only atoms within the neighbor skin distance (see the *neighbor* command) are communicated between processors. You must insure the skin distance is large enough to acquire atoms needed for computing bonds, angles, etc.

A pair style of *none* will also prevent pairwise neighbor lists from being built. However if the *neighbor* style is *bin*, data structures for binning are still allocated. If the neighbor skin distance is small, then these data structures can consume a large amount of memory. So you should either set the neighbor style to *nsq* or set the skin distance to a larger value.

See the *pair_style zero* for a way to trigger the building of a neighbor lists, but compute no pairwise interactions.

18.348.4 Restrictions

none

18.348.5 Related commands

pair_style zero

Default: none

18.349 pair_style oxdna/excv command

18.350 pair_style oxdna/stk command

18.351 pair_style oxdna/hbond command

18.352 pair_style oxdna/xstk command

18.353 pair_style oxdna/coaxstk command

18.353.1 Syntax

```
pair_style style1

pair_coeff * * style2 args
```

- style1 = *hybrid/overlay oxdna/excv oxdna/stk oxdna/hbond oxdna/xstk oxdna/coaxstk*
- style2 = *oxdna/excv* or *oxdna/stk* or *oxdna/hbond* or *oxdna/xstk* or *oxdna/coaxstk*
- args = list of arguments for these particular styles

```
oxdna/stk args = seq T xi kappa 6.0 0.4 0.9 0.32 0.75 1.3 0 0.8 0.9 0 0.95 0.
↪9 0 0.95 2.0 0.65 2.0 0.65
  seq = seqav (for average sequence stacking strength) or seqdep (for␣
↪sequence-dependent stacking strength)
  T = temperature (oxDNA units, 0.1 = 300 K)
  xi = 1.3448 (temperature-independent coefficient in stacking strength)
  kappa = 2.6568 (coefficient of linear temperature dependence in stacking␣
↪strength)
oxdna/hbond args = seq eps 8.0 0.4 0.75 0.34 0.7 1.5 0 0.7 1.5 0 0.7 1.
↪5 0 0.7 0.46 3.141592653589793 0.7 4.0 1.5707963267948966 0.45 4.0 1.
↪5707963267948966 0.45
  seq = seqav (for average sequence base-pairing strength) or seqdep (for␣
↪sequence-dependent base-pairing strength)
  eps = 1.077 (between base pairs A-T and C-G) or 0 (all other pairs)
```

18.353.2 Examples

```
pair_style hybrid/overlay oxdna/excv oxdna/stk oxdna/hbond oxdna/xstk oxdna/coaxstk
pair_coeff * * oxdna/excv    2.0 0.7 0.675 2.0 0.515 0.5 2.0 0.33 0.32
pair_coeff * * oxdna/stk     seqdep 0.1 1.3448 2.6568 6.0 0.4 0.9 0.32 0.75 1.3 0 0.8␣
↪0.9 0 0.95 0.9 0 0.95 2.0 0.65 2.0 0.65
pair_coeff * * oxdna/hbond   seqdep 0.0 8.0 0.4 0.75 0.34 0.7 1.5 0 0.7 1.5 0 0.7 1.5␣
↪0 0.7 0.46 3.141592653589793 0.7 4.0 1.5707963267948966 0.45 4.0 1.5707963267948966␣
↪0.45
pair_coeff 1 4 oxdna/hbond   seqdep 1.077 8.0 0.4 0.75 0.34 0.7 1.5 0 0.7 1.5 0 0.7 1.
↪5 0 0.7 0.46 3.141592653589793 0.7 4.0 1.5707963267948966 0.45 4.0 1.
↪5707963267948966 0.45
pair_coeff 2 3 oxdna/hbond   seqdep 1.077 8.0 0.4 0.75 0.34 0.7 1.5 0 0.7 1.5 0 0.7 1.
↪5 0 0.7 0.46 3.141592653589793 0.7 4.0 1.5707963267948966 0.45 4.0 1.
↪5707963267948966 0.45
```

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```
pair_coeff * * oxdna/xstk    47.5 0.575 0.675 0.495 0.655 2.25 0.791592653589793 0.58␣
↪1.7 1.0 0.68 1.7 1.0 0.68 1.5 0 0.65 1.7 0.875 0.68 1.7 0.875 0.68
pair_coeff * * oxdna/coaxstk 46.0 0.4 0.6 0.22 0.58 2.0 2.541592653589793 0.65 1.3 0␣
↪0.8 0.9 0 0.95 0.9 0 0.95 2.0 -0.65 2.0 -0.65
```

18.353.3 Description

The *oxdna* pair styles compute the pairwise-additive parts of the oxDNA force field for coarse-grained modelling of DNA. The effective interaction between the nucleotides consists of potentials for the excluded volume interaction *oxdna/excv*, the stacking *oxdna/stk*, cross-stacking *oxdna/xstk* and coaxial stacking interaction *oxdna/coaxstk* as well as the hydrogen-bonding interaction *oxdna/hbond* between complementary pairs of nucleotides on opposite strands. Average sequence or sequence-dependent stacking and base-pairing strengths are supported *(Sulc)*. Quasi-unique base-pairing between nucleotides can be achieved by using more complementary pairs of atom types like 5-8 and 6-7, 9-12 and 10-11, 13-16 and 14-15, etc. This prevents the hybridization of in principle complementary bases within Ntypes/4 bases up and down along the backbone.

The exact functional form of the pair styles is rather complex. The individual potentials consist of products of modulation factors, which themselves are constructed from a number of more basic potentials (Morse, Lennard-Jones, harmonic angle and distance) as well as quadratic smoothing and modulation terms. We refer to *(Ouldridge-DPhil)* and *(Ouldridge)* for a detailed description of the oxDNA force field.

Note: These pair styles have to be used together with the related oxDNA bond style *oxdna/fene* for the connectivity of the phosphate backbone (see also documentation of *bond_style oxdna/fene*). Most of the coefficients in the above example have to be kept fixed and cannot be changed without reparameterizing the entire model. Exceptions are the first four coefficients after *oxdna/stk* (seq=seqdep, T=0.1, xi=1.3448 and kappa=2.6568 in the above example) and the first coefficient after *oxdna/hbond* (seq=seqdep in the above example). When using a Langevin thermostat, e.g. through *fix langevin* or *fix nve/dotc/langevin* the temperature coefficients have to be matched to the one used in the fix.

Example input and data files for DNA duplexes can be found in examples/USER/cgdna/examples/oxDNA/ and /oxDNA2/. A simple python setup tool which creates single straight or helical DNA strands, DNA duplexes or arrays of DNA duplexes can be found in examples/USER/cgdna/util/.

Please cite *(Henrich)* in any publication that uses this implementation. The article contains general information on the model, its implementation and performance as well as the structure of the data and input file. The preprint version of the article can be found here. Please cite also the relevant oxDNA publications *(Ouldridge)*, *(Ouldridge-DPhil)* and *(Sulc)*.

18.353.4 Restrictions

These pair styles can only be used if LAMMPS was built with the USER-CGDNA package and the MOLECULE and ASPHERE package. See the *Build package* doc page for more info.

18.353.5 Related commands

bond_style oxdna/fene, *pair_coeff*, *bond_style oxdna2/fene*, *pair_style oxdna2/excv*, *bond_style oxrna2/fene*, *pair_style oxrna2/excv*, *fix nve/dotc/langevin*

Default: none

(Henrich) O. Henrich, Y. A. Gutierrez-Fosado, T. Curk, T. E. Ouldridge, Eur. Phys. J. E 41, 57 (2018).

(Ouldridge-DPhil) T.E. Ouldridge, Coarse-grained modelling of DNA and DNA self-assembly, DPhil. University of Oxford (2011).

(Ouldridge) T.E. Ouldridge, A.A. Louis, J.P.K. Doye, J. Chem. Phys. 134, 085101 (2011).

(Sulc) P. Sulc, F. Romano, T.E. Ouldridge, L. Rovigatti, J.P.K. Doye, A.A. Louis, J. Chem. Phys. 137, 135101 (2012).

18.354 pair_style oxdna2/excv command

18.355 pair_style oxdna2/stk command

18.356 pair_style oxdna2/hbond command

18.357 pair_style oxdna2/xstk command

18.358 pair_style oxdna2/coaxstk command

18.359 pair_style oxdna2/dh command

18.359.1 Syntax

```
pair_style style1

pair_coeff * * style2 args
```

- style1 = *hybrid/overlay oxdna2/excv oxdna2/stk oxdna2/hbond oxdna2/xstk oxdna2/coaxstk oxdna2/dh*
- style2 = *oxdna2/excv* or *oxdna2/stk* or *oxdna2/hbond* or *oxdna2/xstk* or *oxdna2/coaxstk* or *oxdna2/dh*
- args = list of arguments for these particular styles

```
oxdna2/stk args = seq T xi kappa 6.0 0.4 0.9 0.32 0.75 1.3 0 0.8 0.9 0 0.95 0.
↪9 0 0.95 2.0 0.65 2.0 0.65
  seq = seqav (for average sequence stacking strength) or seqdep (for␣
↪sequence-dependent stacking strength)
  T = temperature (oxDNA units, 0.1 = 300 K)
  xi = 1.3523 (temperature-independent coefficient in stacking strength)
  kappa = 2.6717 (coefficient of linear temperature dependence in stacking␣
↪strength)
oxdna2/hbond args = seq eps 8.0 0.4 0.75 0.34 0.7 1.5 0 0.7 1.5 0 0.7 1.
↪5 0 0.7 0.46 3.141592653589793 0.7 4.0 1.5707963267948966 0.45 4.0 1.
↪5707963267948966 0.45
```

```
  seq = seqav (for average sequence base-pairing strength) or seqdep (for␣
↪sequence-dependent base-pairing strength)
  eps = 1.0678 (between base pairs A-T and C-G) or 0 (all other pairs)
oxdna2/dh args = T rhos qeff
  T = temperature (oxDNA units, 0.1 = 300 K)
  rhos = salt concentration (mole per litre)
  qeff = 0.815 (effective charge in elementary charges)
```

18.359.2 Examples

```
pair_style hybrid/overlay oxdna2/excv oxdna2/stk oxdna2/hbond oxdna2/xstk oxdna2/
↪coaxstk oxdna2/dh
pair_coeff * * oxdna2/excv    2.0 0.7 0.675 2.0 0.515 0.5 2.0 0.33 0.32
pair_coeff * * oxdna2/stk     seqdep 0.1 1.3523 2.6717 6.0 0.4 0.9 0.32 0.75 1.3 0 0.
↪8 0.9 0 0.95 0.9 0 0.95 2.0 0.65 2.0 0.65
pair_coeff * * oxdna2/hbond   seqdep 0.0 8.0 0.4 0.75 0.34 0.7 1.5 0 0.7 1.5 0 0.7 1.
↪5 0 0.7 0.46 3.141592653589793 0.7 4.0 1.5707963267948966 0.45 4.0 1.
↪5707963267948966 0.45
pair_coeff 1 4 oxdna2/hbond   seqdep 1.0678 8.0 0.4 0.75 0.34 0.7 1.5 0 0.7 1.5 0 0.7␣
↪1.5 0 0.7 0.46 3.141592653589793 0.7 4.0 1.5707963267948966 0.45 4.0 1.
↪5707963267948966 0.45
pair_coeff 2 3 oxdna2/hbond   seqdep 1.0678 8.0 0.4 0.75 0.34 0.7 1.5 0 0.7 1.5 0 0.7␣
↪1.5 0 0.7 0.46 3.141592653589793 0.7 4.0 1.5707963267948966 0.45 4.0 1.
↪5707963267948966 0.45
pair_coeff * * oxdna2/xstk    47.5 0.575 0.675 0.495 0.655 2.25 0.791592653589793 0.
↪58 1.7 1.0 0.68 1.7 1.0 0.68 1.5 0 0.65 1.7 0.875 0.68 1.7 0.875 0.68
pair_coeff * * oxdna2/coaxstk 58.5 0.4 0.6 0.22 0.58 2.0 2.891592653589793 0.65 1.3 0␣
↪0.8 0.9 0 0.95 0.9 0 0.95 40.0 3.116592653589793
pair_coeff * * oxdna2/dh      0.1 0.5 0.815
```

18.359.3 Description

The *oxdna2* pair styles compute the pairwise-additive parts of the oxDNA force field for coarse-grained modelling of DNA. The effective interaction between the nucleotides consists of potentials for the excluded volume interaction *oxdna2/excv*, the stacking *oxdna2/stk*, cross-stacking *oxdna2/xstk* and coaxial stacking interaction *oxdna2/coaxstk*, electrostatic Debye-Hueckel interaction *oxdna2/dh* as well as the hydrogen-bonding interaction *oxdna2/hbond* between complementary pairs of nucleotides on opposite strands. Average sequence or sequence-dependent stacking and base-pairing strengths are supported *(Sulc)*. Quasi-unique base-pairing between nucleotides can be achieved by using more complementary pairs of atom types like 5-8 and 6-7, 9-12 and 10-11, 13-16 and 14-15, etc. This prevents the hybridization of in principle complementary bases within Ntypes/4 bases up and down along the backbone.

The exact functional form of the pair styles is rather complex. The individual potentials consist of products of modulation factors, which themselves are constructed from a number of more basic potentials (Morse, Lennard-Jones, harmonic angle and distance) as well as quadratic smoothing and modulation terms. We refer to *(Snodin)* and the original oxDNA publications *(Ouldridge-DPhil)* and *(Ouldridge)* for a detailed description of the oxDNA2 force field.

Note: These pair styles have to be used together with the related oxDNA2 bond style *oxdna2/fene* for the connectivity of the phosphate backbone (see also documentation of *bond_style oxdna2/fene*). Most of the coefficients in the above example have to be kept fixed and cannot be changed without reparameterizing the entire model. Exceptions are the first four coefficients after *oxdna2/stk* (seq=seqdep, T=0.1, xi=1.3523 and kappa=2.6717 in the above example), the first coefficient after *oxdna2/hbond* (seq=seqdep in the above example) and the three coefficients after *oxdna2/dh* (T=0.1, rhos=0.5, qeff=0.815 in the above example). When using a Langevin thermostat e.g. through *fix langevin* or

fix nve/dotc/langevin the temperature coefficients have to be matched to the one used in the fix.

Example input and data files for DNA duplexes can be found in examples/USER/cgdna/examples/oxDNA/ and /oxDNA2/. A simple python setup tool which creates single straight or helical DNA strands, DNA duplexes or arrays of DNA duplexes can be found in examples/USER/cgdna/util/.

Please cite *(Henrich)* in any publication that uses this implementation. The article contains general information on the model, its implementation and performance as well as the structure of the data and input file. The preprint version of the article can be found here. Please cite also the relevant oxDNA2 publications *(Snodin)* and *(Sulc)*.

18.359.4 Restrictions

These pair styles can only be used if LAMMPS was built with the USER-CGDNA package and the MOLECULE and ASPHERE package. See the *Build package* doc page for more info.

18.359.5 Related commands

bond_style oxdna2/fene, *pair_coeff* , *bond_style oxdna/fene*, *pair_style oxdna/excv*, *bond_style oxrna2/fene*, *pair_style oxrna2/excv*, *fix nve/dotc/langevin*

Default: none

(Henrich) O. Henrich, Y. A. Gutierrez-Fosado, T. Curk, T. E. Ouldridge, Eur. Phys. J. E 41, 57 (2018).

(Snodin) B.E. Snodin, F. Randisi, M. Mosayebi, et al., J. Chem. Phys. 142, 234901 (2015).

(Sulc) P. Sulc, F. Romano, T.E. Ouldridge, L. Rovigatti, J.P.K. Doye, A.A. Louis, J. Chem. Phys. 137, 135101 (2012).

(Ouldridge-DPhil) T.E. Ouldridge, Coarse-grained modelling of DNA and DNA self-assembly, DPhil. University of Oxford (2011).

(Ouldridge) T.E. Ouldridge, A.A. Louis, J.P.K. Doye, J. Chem. Phys. 134, 085101 (2011).

18.360 pair_style oxrna2/excv command

18.361 pair_style oxrna2/stk command

18.362 pair_style oxrna2/hbond command

18.363 pair_style oxrna2/xstk command

18.364 pair_style oxrna2/coaxstk command

18.365 pair_style oxrna2/dh command

18.365.1 Syntax

```
pair_style style1

pair_coeff * * style2 args
```

- style1 = *hybrid/overlay oxrna2/excv oxrna2/stk oxrna2/hbond oxrna2/xstk oxrna2/coaxstk oxrna2/dh*
- style2 = *oxrna2/excv* or *oxrna2/stk* or *oxrna2/hbond* or *oxrna2/xstk* or *oxrna2/coaxstk* or *oxrna2/dh*
- args = list of arguments for these particular styles

```
oxrna2/stk args = seq T xi kappa 6.0 0.43 0.93 0.35 0.78 0.9 0 0.95 0.9 0 0.
↪95 1.3 0 0.8 1.3 0 0.8 2.0 0.65 2.0 0.65
  seq = seqav (for average sequence stacking strength) or seqdep (for␣
↪sequence-dependent stacking strength)
  T = temperature (oxDNA units, 0.1 = 300 K)
  xi = 1.40206 (temperature-independent coefficient in stacking strength)
  kappa = 2.77 (coefficient of linear temperature dependence in stacking␣
↪strength)
oxrna2/hbond args = seq eps 8.0 0.4 0.75 0.34 0.7 1.5 0 0.7 1.5 0 0.7 1.
↪5 0 0.7 0.46 3.141592653589793 0.7 4.0 1.5707963267948966 0.45 4.0 1.
↪5707963267948966 0.45
  seq = seqav (for average sequence base-pairing strength) or seqdep (for␣
↪sequence-dependent base-pairing strength)
  eps = 0.870439 (between base pairs A-T, C-G and G-T) or 0 (all other pairs)
oxrna2/dh args = T rhos qeff
  T = temperature (oxDNA units, 0.1 = 300 K)
  rhos = salt concentration (mole per litre)
  qeff = 1.02455 (effective charge in elementary charges)
```

18.365.2 Examples

```
pair_style hybrid/overlay oxrna2/excv oxrna2/stk oxrna2/hbond oxrna2/xstk oxrna2/
↪coaxstk oxrna2/dh
pair_coeff * * oxrna2/excv    2.0 0.7 0.675 2.0 0.515 0.5 2.0 0.33 0.32
pair_coeff * * oxrna2/stk     seqdep 0.1 1.40206 2.77 6.0 0.43 0.93 0.35 0.78 0.9 0 0.
↪95 0.9 0 0.95 1.3 0 0.8 1.3 0 0.8 2.0 0.65 2.0 0.65
pair_coeff * * oxrna2/hbond   seqdep 0.0 8.0 0.4 0.75 0.34 0.7 1.5 0 0.7 1.5 0 0.7 1.
↪5 0 0.7 0.46 3.141592653589793 0.7 4.0 1.5707963267948966 0.45 4.0 1.
↪5707963267948966 0.45
pair_coeff 1 4 oxrna2/hbond   seqdep 0.870439 8.0 0.4 0.75 0.34 0.7 1.5 0 0.7 1.5 0 0.
↪7 1.5 0 0.7 0.46 3.141592653589793 0.7 4.0 1.5707963267948966 0.45 4.0 1.
↪5707963267948966 0.45
pair_coeff 2 3 oxrna2/hbond   seqdep 0.870439 8.0 0.4 0.75 0.34 0.7 1.5 0 0.7 1.5 0 0.
↪7 1.5 0 0.7 0.46 3.141592653589793 0.7 4.0 1.5707963267948966 0.45 4.0 1.
↪5707963267948966 0.45
pair_coeff 3 4 oxrna2/hbond   seqdep 0.870439 8.0 0.4 0.75 0.34 0.7 1.5 0 0.7 1.5 0 0.
↪7 1.5 0 0.7 0.46 3.141592653589793 0.7 4.0 1.5707963267948966 0.45 4.0 1.
↪5707963267948966 0.45
pair_coeff * * oxrna2/xstk    59.9626 0.5 0.6 0.42 0.58 2.25 0.505 0.58 1.7 1.266 0.
↪68 1.7 1.266 0.68 1.7 0.309 0.68 1.7 0.309 0.68
pair_coeff * * oxrna2/coaxstk 80 0.5 0.6 0.42 0.58 2.0 2.592 0.65 1.3 0.151 0.8 0.9 0.
↪685 0.95 0.9 0.685 0.95 2.0 -0.65 2.0 -0.65
pair_coeff * * oxrna2/dh      0.1 0.5 1.02455
```

18.365.3 Description

The *oxrna2* pair styles compute the pairwise-additive parts of the oxDNA force field for coarse-grained modelling of DNA. The effective interaction between the nucleotides consists of potentials for the excluded volume interaction *oxrna2/excv*, the stacking *oxrna2/stk*, cross-stacking *oxrna2/xstk* and coaxial stacking interaction *oxrna2/coaxstk*, electrostatic Debye-Hueckel interaction *oxrna2/dh* as well as the hydrogen-bonding interaction *oxrna2/hbond* between complementary pairs of nucleotides on opposite strands. Average sequence or sequence-dependent stacking and base-pairing strengths are supported *(Sulc2)*. Quasi-unique base-pairing between nucleotides can be achieved by using more complementary pairs of atom types like 5-8 and 6-7, 9-12 and 10-11, 13-16 and 14-15, etc. This prevents the hybridization of in principle complementary bases within Ntypes/4 bases up and down along the backbone.

The exact functional form of the pair styles is rather complex. The individual potentials consist of products of modulation factors, which themselves are constructed from a number of more basic potentials (Morse, Lennard-Jones, harmonic angle and distance) as well as quadratic smoothing and modulation terms. We refer to *(Sulc1)* and the original oxDNA publications *(Ouldridge-DPhil)* and *(Ouldridge)* for a detailed description of the oxRNA2 force field.

Note: These pair styles have to be used together with the related oxDNA2 bond style *oxrna2/fene* for the connectivity of the phosphate backbone (see also documentation of *bond_style oxrna2/fene*). Most of the coefficients in the above example have to be kept fixed and cannot be changed without reparameterizing the entire model. Exceptions are the first four coefficients after *oxrna2/stk* (seq=seqdep, T=0.1, xi=1.40206 and kappa=2.77 in the above example), the first coefficient after *oxrna2/hbond* (seq=seqdep in the above example) and the three coefficients after *oxrna2/dh* (T=0.1, rhos=0.5, qeff=1.02455 in the above example). When using a Langevin thermostat e.g. through *fix langevin* or *fix nve/dotc/langevin* the temperature coefficients have to be matched to the one used in the fix.

Example input and data files for DNA duplexes can be found in examples/USER/cgdna/examples/oxDNA/ and /oxDNA2/. A simple python setup tool which creates single straight or helical DNA strands, DNA duplexes or arrays of DNA duplexes can be found in examples/USER/cgdna/util/.

Please cite *(Henrich)* in any publication that uses this implementation. The article contains general information on the

model, its implementation and performance as well as the structure of the data and input file. The preprint version of the article can be found here. Please cite also the relevant oxRNA2 publications *(Sulc1)* and *(Sulc2)*.

18.365.4 Restrictions

These pair styles can only be used if LAMMPS was built with the USER-CGDNA package and the MOLECULE and ASPHERE package. See the *Build package* doc page for more info.

18.365.5 Related commands

bond_style oxrna2/fene, *pair_coeff*, *bond_style oxdna/fene*, *pair_style oxdna/excv*, *bond_style oxdna2/fene*, *pair_style oxdna2/excv*, *fix nve/dotc/langevin*

Default:

none

(Henrich) O. Henrich, Y. A. Gutierrez-Fosado, T. Curk, T. E. Ouldridge, Eur. Phys. J. E 41, 57 (2018).

(Sulc1) P. Sulc, F. Romano, T. E. Ouldridge, et al., J. Chem. Phys. 140, 235102 (2014).

(Sulc2) P. Sulc, F. Romano, T.E. Ouldridge, L. Rovigatti, J.P.K. Doye, A.A. Louis, J. Chem. Phys. 137, 135101 (2012).

(Ouldridge-DPhil) T.E. Ouldridge, Coarse-grained modelling of DNA and DNA self-assembly, DPhil. University of Oxford (2011).

(Ouldridge) T.E. Ouldridge, A.A. Louis, J.P.K. Doye, J. Chem. Phys. 134, 085101 (2011).

18.366 pair_style peri/pmb command

18.367 pair_style peri/pmb/omp command

18.368 pair_style peri/lps command

18.369 pair_style peri/lps/omp command

18.370 pair_style peri/ves command

18.371 pair_style peri/eps command

18.371.1 Syntax

```
pair_style style
```

- style = *peri/pmb* or *peri/lps* or *peri/ves* or *peri/eps*

18.371.2 Examples

```
pair_style peri/pmb
pair_coeff * * 1.6863e22 0.0015001 0.0005 0.25

pair_style peri/lps
pair_coeff * * 14.9e9 14.9e9 0.0015001 0.0005 0.25

pair_style peri/ves
pair_coeff * * 14.9e9 14.9e9 0.0015001 0.0005 0.25 0.5 0.001

pair_style peri/eps
pair_coeff * * 14.9e9 14.9e9 0.0015001 0.0005 0.25 118.43
```

18.371.3 Description

The peridynamic pair styles implement material models that can be used at the mesoscopic and macroscopic scales. See this document for an overview of LAMMPS commands for Peridynamics modeling.

Style *peri/pmb* implements the Peridynamic bond-based prototype microelastic brittle (PMB) model.

Style *peri/lps* implements the Peridynamic state-based linear peridynamic solid (LPS) model.

Style *peri/ves* implements the Peridynamic state-based linear peridynamic viscoelastic solid (VES) model.

Style *peri/eps* implements the Peridynamic state-based elastic-plastic solid (EPS) model.

The canonical papers on Peridynamics are *(Silling 2000)* and *(Silling 2007)*. The implementation of Peridynamics in LAMMPS is described in *(Parks)*. Also see the PDLAMMPS user guide for more details about its implementation.

The peridynamic VES and EPS models in PDLAMMPS were implemented by R. Rahman and J. T. Foster at University of Texas at San Antonio. The original VES formulation is described in "(Mitchell2011)" and the original EPS formulation is in "(Mitchell2011a)". Additional PDF docs that describe the VES and EPS implementations are include in the LAMMPS distribution in doc/PDF/PDLammps_VES.pdf and doc/PDF/PDLammps_EPS.pdf. For questions regarding the VES and EPS models in LAMMPS you can contact R. Rahman (rezwanur.rahman at utsa.edu).

The following coefficients must be defined for each pair of atom types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below.

For the *peri/pmb* style:

- c (energy/distance/volume^2 units)
- horizon (distance units)
- s00 (unitless)
- α (unitless)

C is the effectively a spring constant for Peridynamic bonds, the horizon is a cutoff distance for truncating interactions, and s00 and α are used as a bond breaking criteria. The units of c are such that c/distance = stiffness/volume^2, where stiffness is energy/distance^2 and volume is distance^3. See the users guide for more details.

For the *peri/lps* style:

- K (force/area units)
- G (force/area units)
- horizon (distance units)

- s00 (unitless)
- α (unitless)

K is the bulk modulus and G is the shear modulus. The horizon is a cutoff distance for truncating interactions, and s00 and α are used as a bond breaking criteria. See the users guide for more details.

For the *peri/ves* style:

- K (force/area units)
- G (force/area units)
- horizon (distance units)
- s00 (unitless)
- α (unitless)
- m_lambdai (unitless)
- m_taubi (unitless)

K is the bulk modulus and G is the shear modulus. The horizon is a cutoff distance for truncating interactions, and s00 and α are used as a bond breaking criteria. m_lambdai and m_taubi are the viscoelastic relaxation parameter and time constant, respectively. m_lambdai varies within zero to one. For very small values of m_lambdai the viscoelastic model responds very similar to a linear elastic model. For details please see the description in "(Mtchell2011)".

For the *peri/eps* style:

- K (force/area units)
- G (force/area units)
- horizon (distance units)
- s00 (unitless)
- α (unitless)
- m_yield_stress (force/area units)

K is the bulk modulus and G is the shear modulus. The horizon is a cutoff distance and s00 and α are used as a bond breaking criteria. m_yield_stress is the yield stress of the material. For details please see the description in "(Mtchell2011a)".

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

These pair styles do not support the *pair_modify* shift option.

The *pair_modify* table and tail options are not relevant for these pair styles.

These pair styles write their information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the *run_style respa* command. They do not support the *inner*, *middle*, *outer* keywords.

18.371.4 Restrictions

All of these styles are part of the PERI package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.371.5 Related commands

pair_coeff

Default: none

(Parks) Parks, Lehoucq, Plimpton, Silling, Comp Phys Comm, 179(11), 777-783 (2008).

(Silling 2000) Silling, J Mech Phys Solids, 48, 175-209 (2000).

(Silling 2007) Silling, Epton, Weckner, Xu, Askari, J Elasticity, 88, 151-184 (2007).

(Mitchell2011) Mitchell. A non-local, ordinary-state-based viscoelasticity model for peridynamics. Sandia National Lab Report, 8064:1-28 (2011).

(Mitchell2011a) Mitchell. A Nonlocal, Ordinary, State-Based Plasticity Model for Peridynamics. Sandia National Lab Report, 3166:1-34 (2011).

18.372 pair_style polymorphic command

18.372.1 Syntax

```
pair_style polymorphic
```

style = *polymorphic*

18.372.2 Examples

```
pair_style polymorphic
pair_coeff * * TlBr_msw.polymorphic Tl Br
pair_coeff * * AlCu_eam.polymorphic Al Cu
pair_coeff * * GaN_tersoff.polymorphic Ga N
pair_coeff * * GaN_sw.polymorphic GaN
```

18.372.3 Description

The *polymorphic* pair style computes a 3-body free-form potential (*Zhou*) for the energy E of a system of atoms as

$$E = \frac{1}{2} \sum_{i=1}^{i=N} \sum_{j=1}^{j=N} \left[(1-\delta_{ij}) \cdot U_{IJ}\left(r_{ij}\right) - (1-\eta_{ij}) \cdot F_{IJ}\left(r_{ij}\right) \cdot V_{IJ}\left(r_{ij}\right) \right]$$

$$X_{ij} = \sum_{k=i_1, k \neq i,j}^{i_N} W_{IK}\left(r_{ik}\right) \cdot G_{JIK}\left(\theta_{jik}\right) \cdot P_{IK}\left(\Delta r_{jik}\right)$$

$$\Delta r_{jik} = r_{ij} - \xi_{IJ} \cdot r_{ik}$$

where I, J, K represent species of atoms i, j, and k, $i_1, ..., i_N$ represents a list of i's neighbors, δ_{ij} is a Dirac constant (i.e., $\delta_{ij} = 1$ when $i = j$, and $\delta_{ij} = 0$ otherwise), η_{ij} is similar constant that can be set either to $\eta_{ij} = \delta_{ij}$ or $\eta_{ij} = 1 - \delta_{ij}$ depending on the potential type, $U_{IJ}(r_{ij})$, $V_{IJ}(r_{ij})$, $W_{IK}(r_{ik})$ are pair functions, $G_{JIK}(\cos(\theta))$ is an angular function, $P_{IK}(\Delta r_{jik})$ is a function of atomic spacing differential $\Delta r_{jik} = r_{ij} - \xi_{IJ} \cdot r_{ik}$ with ξ_{IJ} being a pair-dependent parameter, and $F_{IJ}(X_{ij})$ is a function of the local environment variable X_{ij}. This generic potential is fully defined once the constants η_{ij} and ξ_{IJ}, and the six functions $U_{IJ}(r_{ij})$, $V_{IJ}(r_{ij})$, $W_{IK}(r_{ik})$, $G_{JIK}(\cos(\theta))$, $P_{IK}(\Delta r_{jik})$, and $F_{IJ}(X_{ij})$ are given. Note that these six functions are all one dimensional, and hence can be provided in an analytic or tabular form. This allows users to design different potentials solely based on a manipulation of these functions. For instance, the potential reduces to Stillinger-Weber potential (*SW*) if we set

$$\begin{cases} \eta_{ij} = \delta_{ij}, \xi_{IJ} = 0 \\ U_{IJ}\left(r\right) = A_{IJ} \cdot \epsilon_{IJ} \cdot \left(\frac{\sigma_{IJ}}{r}\right)^q \cdot \left[B_{IJ} \cdot \left(\frac{\sigma_{IJ}}{r}\right)^{p-q} - 1\right] \cdot exp\left(\frac{\sigma_{IJ}}{r - a_{IJ} \cdot \sigma_{IJ}}\right) \\ V_{IJ}\left(r\right) = \sqrt{\lambda_{IJ} \cdot \epsilon_{IJ}} \cdot exp\left(\frac{\gamma_{IJ} \cdot \sigma_{IJ}}{r - a_{IJ} \cdot \sigma_{IJ}}\right) \\ F_{IJ}\left(X\right) = -X \\ P_{IJ}\left(\Delta r\right) = 1 \\ W_{IJ}\left(r\right) = \sqrt{\lambda_{IJ} \cdot \epsilon_{IJ}} \cdot exp\left(\frac{\gamma_{IJ} \cdot \sigma_{IJ}}{r - a_{IJ} \cdot \sigma_{IJ}}\right) \\ G_{JIK}\left(\theta\right) = \left(cos\theta + \frac{1}{3}\right)^2 \end{cases}$$

The potential reduces to Tersoff types of potential (*Tersoff* or *Albe*) if we set

$$\begin{cases} \eta_{ij} = \delta_{ij}, \xi_{IJ} = 1 \\ U_{IJ}\left(r\right) = \frac{D_{e,IJ}}{S_{IJ}-1} \cdot exp\left[-\beta_{IJ}\sqrt{2S_{IJ}\left(r - r_{e,IJ}\right)}\right] \cdot f_{c,IJ}\left(r\right) \\ V_{IJ}\left(r\right) = \frac{S_{IJ} \cdot D_{e,IJ}}{S_{IJ}-1} \cdot exp\left[-\beta_{IJ}\sqrt{\frac{2}{S_{IJ}}\left(r - r_{e,IJ}\right)}\right] \cdot f_{c,IJ}\left(r\right) \\ F_{IJ}\left(X\right) = \left(1 + X\right)^{-\frac{1}{2}} \\ P_{IJ}\left(\Delta r\right) = exp\left(2\mu_{IK} \cdot \Delta r\right) \\ W_{IJ}\left(r\right) = f_{c,IK}\left(r\right) \\ G_{JIK}\left(\theta\right) = \gamma_{IK}\left[1 + \frac{c_{IK}^2}{d_{IK}^2} - \frac{c_{IK}^2}{d_{IK}^2 + \left(h_{IK} + cos\theta\right)^2}\right] \end{cases}$$

$$f_{c,IJ} = \begin{cases} 1, & r \leq r_{s,IJ} \\ \frac{1}{2} + \frac{1}{2}cos\left[\frac{\pi\left(r - r_{s,IJ}\right)}{r_{c,IJ} - r_{s,IJ}}\right], & r_{s,IJ} < r < r_{c,IJ} \\ 0, & r \geq r_{c,IJ} \end{cases}$$

The potential reduces to Rockett-Tersoff (*Wang*) type if we set

$$\begin{cases} \eta_{ij} = \delta_{ij}, \xi_{IJ} = 1 \\ U_{IJ}(r) = \begin{cases} A_{IJ} \cdot exp(-\lambda_{1,IJ} \cdot r) \cdot f_{c,IJ}(r), & r \le r_{s,1,IJ} \\ A_{IJ} \cdot exp(-\lambda_{1,IJ} \cdot r) \cdot f_{c,IJ}(r) \cdot f_{c,1,IJ}(r), & r_{s,1,IJ} < r < r_{c,1,IJ} \\ 0, & r \ge r_{c,1,IJ} \end{cases} \\ V_{IJ}(r) = \begin{cases} B_{IJ} \cdot exp(-\lambda_{2,IJ} \cdot r) \cdot f_{c,IJ}(r), & r \le r_{s,1,IJ} \\ B_{IJ} \cdot exp(-\lambda_{2,IJ} \cdot r) \cdot f_{c,IJ}(r) + A_{IJ} \cdot exp(-\lambda_{1,IJ} \cdot r) \cdot \\ \quad f_{c,IJ}(r) \cdot [1 - f_{c,1,IJ}(r)], & r_{s,1,IJ} < r < r_{c,1,IJ} \\ B_{IJ} \cdot exp(-\lambda_{2,IJ} \cdot r) \cdot f_{c,IJ}(r) + A_{IJ} \cdot exp(-\lambda_{1,IJ} \cdot r) \cdot \\ \quad f_{c,IJ}(r) & r \ge r_{c,1,IJ} \end{cases} \\ F_{IJ}(X) = [1 + (\beta_{IJ} \cdot X)^{n_{IJ}}]^{-\frac{1}{2n_{IJ}}} \\ P_{IJ}(\Delta r) = exp\left(\lambda_{3,IK} \cdot \Delta r^3\right) \\ W_{IJ}(r) = f_{c,IK}(r) \\ G_{JIK}(\theta) = 1 + \frac{c_{IK}^2}{d_{IK}^2} - \frac{c_{IK}^2}{d_{IK}^2 + (h_{IK} + cos\theta)^2} \end{cases}$$

$$f_{c,IJ} = \begin{cases} 1, & r \le r_{s,IJ} \\ \frac{1}{2} + \frac{1}{2} cos\left[\frac{\pi(r - r_{s,IJ})}{r_{c,IJ} - r_{s,IJ}}\right], & r_{s,IJ} < r < r_{c,IJ} \\ 0, & r \ge r_{c,IJ} \end{cases}$$

$$f_{c,1,IJ} = \begin{cases} 1, & r \le r_{s,1,IJ} \\ \frac{1}{2} + \frac{1}{2} cos\left[\frac{\pi(r - r_{s,1,IJ})}{r_{c,1,IJ} - r_{s,1,IJ}}\right], & r_{s,1,IJ} < r < r_{c,1,IJ} \\ 0, & r \ge r_{c,1,IJ} \end{cases}$$

The potential becomes embedded atom method (*Daw*) if we set

$$\begin{cases} \eta_{ij} = 1 - \delta_{ij}, \xi_{IJ} = 0 \\ U_{IJ}(r) = \phi_{IJ}(r) \\ V_{IJ}(r) = 1 \\ F_{II}(X) = -2F_I(X) \\ P_{IJ}(\Delta r) = 1 \\ W_{IJ}(r) = f_K(r) \\ G_{JIK}(\theta) = 1 \end{cases}$$

In the embedded atom method case, $\phi_{IJ}(r_{ij})$ is the pair energy, $F_I(X)$ is the embedding energy, *X* is the local electron density, and $f_K(r)$ is the atomic electron density function.

If the tabulated functions are created using the parameters of sw, tersoff, and eam potentials, the polymorphic pair style will produce the same global properties (energies and stresses) and the same forces as the sw, tersoff, and eam pair styles. The polymorphic pair style also produces the same atom properties (energies and stresses) as the corresponding tersoff and eam pair styles. However, due to a different partition of global properties to atom properties, the polymorphic pair style will produce different atom properties (energies and stresses) as the sw pair style. This does not mean that polymorphic pair style is different from the sw pair style in this case. It just means that the definitions of the atom energies and atom stresses are different.

Only a single pair_coeff command is used with the polymorphic style which specifies an potential file for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of Tersoff elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential file. Several files for polymorphic potentials are included in the potentials directory of the LAMMPS distribution. They have a "poly" suffix.

As an example, imagine the SiC_tersoff.poly file has tabulated functions for Si-C tersoff potential. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * SiC_tersoff.poly Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the polymorphic file. The final C argument maps LAMMPS atom type 4 to the C element in the polymorphic file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when an polymorphic potential is used as part of the hybrid pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Potential files in the potentials directory of the LAMMPS distribution have a ".poly" suffix. At the beginning of the files, an unlimited number of lines starting with '#' are used to describe the potential and are ignored by LAMMPS. The next line lists two numbers:

ntypes η

Here ntypes represent total number of species defined in the potential file, and $\eta = 0$ or 1. The number ntypes must equal the total number of different species defined in the pair_coeff command. When $\eta = 1$, :math:eta_{ij}` defined in the potential functions above is set to $1 - \delta_{ij}$, otherwise η_{ij} is set to δ_{ij}. The next ntypes lines each lists two numbers and a character string representing atomic number, atomic mass, and name of the species of the ntypes elements:

```
atomic_number atomic-mass element (1)
atomic_number atomic-mass element (2)
...
atomic_number atomic-mass element (ntypes)
```

The next ntypes*(ntypes+1)/2 lines contain two numbers:

cut xi (1)
cut xi (2)
...
cut xi (ntypes*(ntypes+1)/2)

Here cut means the cutoff distance of the pair functions, ξ is the same as defined in the potential functions above. The ntypes*(ntypes+1)/2 lines are related to the pairs according to the sequence of first ii (self) pairs, i = 1, 2, . . . , ntypes, and then then ij (cross) pairs, i = 1, 2, . . . , ntypes-1, and j = i+1, i+2, . . . , ntypes (i.e., the sequence of the ij pairs follows 11, 22, . . . , 12, 13, 14, . . . , 23, 24, . . .).

The final blocks of the potential file are the U, V, W, P, G, and F functions are listed sequentially. First, U functions are given for each of the ntypes*(ntypes+1)/2 pairs according to the sequence described above. For each of the pairs, nr values are listed. Next, similar arrays are given for V, W, and P functions. Then G functions are given for all the ntypes*ntypes*ntypes ijk triplets in a natural sequence i from 1 to ntypes, j from 1 to ntypes, and k from 1 to ntypes (i.e., ijk = 111, 112, 113, . . . , 121, 122, 123 . . . , 211, 212, . . .). Each of the ijk functions contains ng values. Finally, the F functions are listed for all ntypes*(ntypes+1)/2 pairs, each containing nx values. Either analytic or tabulated functions can be specified. Currently, constant, exponential, sine and cosine analytic functions are available which are specified with: constant c1 , where f(x) = c1 exponential c1 c2 , where f(x) = c1 exp(c2*x) sine c1 c2 , where f(x) = c1 sin(c2*x) cos c1 c2 , where f(x) = c1 cos(c2*x) Tabulated functions are specified by spline n x1 x2, where n=number of point, (x1,x2)=range and then followed by n values evaluated uniformly over these argument ranges. The valid argument ranges of the functions are between 0 <= r <= cut for the U(r), V(r), W(r) functions, -cutmax <= delta_r <= cutmax for the P(delta_r) functions, -1 <= $\cos\theta$ <= 1 for the G($\cos\theta$) functions, and 0 <= X <= maxX for the F(X) functions.

Mixing, shift, table tail correction, restart:

This pair styles does not support the *pair_modify* shift, table, and tail options.

This pair style does not write their information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

18.372.4 Restrictions

If using create_atoms command, atomic masses must be defined in the input script. If using read_data, atomic masses must be defined in the atomic structure data file.

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This pair potential requires the *newton* setting to be "on" for pair interactions.

The potential files provided with LAMMPS (see the potentials directory) are parameterized for metal *units*. You can use any LAMMPS units, but you would need to create your own potential files.

18.372.5 Related commands

pair_coeff

(Zhou) X. W. Zhou, M. E. Foster, R. E. Jones, P. Yang, H. Fan, and F. P. Doty, J. Mater. Sci. Res., 4, 15 (2015).

(SW) F. H. Stillinger-Weber, and T. A. Weber, Phys. Rev. B, 31, 5262 (1985).

(Tersoff) J. Tersoff, Phys. Rev. B, 39, 5566 (1989).

(Albe) K. Albe, K. Nordlund, J. Nord, and A. Kuronen, Phys. Rev. B, 66, 035205 (2002).

(Wang) J. Wang, and A. Rockett, Phys. Rev. B, 43, 12571 (1991).

(Daw) M. S. Daw, and M. I. Baskes, Phys. Rev. B, 29, 6443 (1984).

18.373 pair_style python command

18.373.1 Syntax

```
pair_style python cutoff
```

cutoff = global cutoff for interactions in python potential classes

18.373.2 Examples

```
pair_style python 2.5
pair_coeff * * py_pot.LJCutMelt lj

pair_style hybrid/overlay coul/long 12.0 python 12.0
pair_coeff * * coul/long
pair_coeff * * python py_pot.LJCutSPCE OW NULL
```

18.373.3 Description

The *python* pair style provides a way to define pairwise additive potential functions as python script code that is loaded into LAMMPS from a python file which must contain specific python class definitions. This allows to rapidly evaluate different potential functions without having to modify and re-compile LAMMPS. Due to python being an interpreted language, however, the performance of this pair style is going to be significantly slower (often between 20x and 100x) than corresponding compiled code. This penalty can be significantly reduced through generating tabulations from the python code through the *pair_write* command, which is supported by this style.

Only a single pair_coeff command is used with the *python* pair style which specifies a python class inside a python module or file that LAMMPS will look up in the current directory, the folder pointed to by the LAMMPS_POTENTIALS environment variable or somewhere in your python path. A single python module can hold multiple python pair class definitions. The class definitions itself have to follow specific rules that are explained below.

Atom types in the python class are specified through symbolic constants, typically strings. These are mapped to LAMMPS atom types by specifying N additional arguments after the class name in the pair_coeff command, where N must be the number of currently defined atom types:

As an example, imagine a file *py_pot.py* has a python potential class names *LJCutMelt* with parameters and potential functions for a two Lennard-Jones atom types labeled as 'LJ1' and 'LJ2'. In your LAMMPS input and you would have defined 3 atom types, out of which the first two are supposed to be using the 'LJ1' parameters and the third the 'LJ2' parameters, then you would use the following pair_coeff command:

```
pair_coeff * * py_pot.LJCutMelt LJ1 LJ1 LJ2
```

The first two arguments **must** be * * so as to span all LAMMPS atom types. The first two LJ1 arguments map LAMMPS atom types 1 and 2 to the LJ1 atom type in the LJCutMelt class of the py_pot.py file. The final LJ2 argument maps LAMMPS atom type 3 to the LJ2 atom type the python file. If a mapping value is specified as NULL, the mapping is not performed, any pair interaction with this atom type will be skipped. This can be used when a *python* potential is used as part of the *hybrid* or *hybrid/overlay* pair style. The NULL values are then placeholders for atom types that will be used with other potentials.

The python potential file has to start with the following code:

```
from __future__ import print_function

class LAMMPSPairPotential(object):
    def __init__(self):
        self.pmap=dict()
        self.units='lj'
    def map_coeff(self,name,ltype):
        self.pmap[ltype]=name
    def check_units(self,units):
        if (units != self.units):
           raise Exception("Conflicting units: %s vs. %s" % (self.units,units))
```

Any classes with definitions of specific potentials have to be derived from this class and should be initialize in a similar fashion to the example given below.

Note: The class constructor has to set up a data structure containing the potential parameters supported by this class. It should also define a variable *self.units* containing a string matching one of the options of LAMMPS' *units* command, which is used to verify, that the potential definition in the python class and in the LAMMPS input match.

Here is an example for a single type Lennard-Jones potential class *LJCutMelt* in reduced units, which defines an atom type *lj* for which the parameters epsilon and sigma are both 1.0:

```
class LJCutMelt(LAMMPSPairPotential):
    def __init__(self):
        super(LJCutMelt,self).__init__()
        # set coeffs: 48\*eps\*sig\*\*12, 24\*eps\*sig\*\*6,
        #              4\*eps\*sig\*\*12,  4\*eps\*sig\*\*6
        self.units = 'lj'
        self.coeff = {'lj'  : {'lj'  : (48.0,24.0,4.0,4.0)}}
```

The class also has to provide two methods for the computation of the potential energy and forces, which have be named *compute_force*, and *compute_energy*, which both take 3 numerical arguments:

- rsq = the square of the distance between a pair of atoms (float)
- itype = the (numerical) type of the first atom
- jtype = the (numerical) type of the second atom

This functions need to compute the force and the energy, respectively, and use the result as return value. The functions need to use the *pmap* dictionary to convert the LAMMPS atom type number to the symbolic value of the internal potential parameter data structure. Following the *LJCutMelt* example, here are the two functions:

```
def compute_force(self,rsq,itype,jtype):
     coeff = self.coeff[self.pmap[itype]][self.pmap[jtype]]
     r2inv  = 1.0/rsq
     r6inv  = r2inv\*r2inv\*r2inv
     lj1 = coeff[0]
     lj2 = coeff[1]
     return (r6inv \* (lj1\*r6inv - lj2))\*r2inv

 def compute_energy(self,rsq,itype,jtype):
     coeff = self.coeff[self.pmap[itype]][self.pmap[jtype]]
     r2inv  = 1.0/rsq
     r6inv  = r2inv\*r2inv\*r2inv
     lj3 = coeff[2]
     lj4 = coeff[3]
     return (r6inv \* (lj3\*r6inv - lj4))
```

Note: for consistency with the C++ pair styles in LAMMPS, the *compute_force* function follows the conventions of the Pair::single() methods and does not return the full force, but the force scaled by the distance between the two atoms, so this value only needs to be multiplied by delta x, delta y, and delta z to conveniently obtain the three components of the force vector between these two atoms.

Note: The evaluation of scripted python code will slow down the computation pair-wise interactions quite significantly. However, this can be largely worked around through using the python pair style not for the actual simulation, but to generate tabulated potentials on the fly using the *pair_write* command. Please see below for an example LAMMPS input of how to build a table file:

```
pair_style python 2.5
pair_coeff * * py_pot.LJCutMelt lj
shell rm -f melt.table
pair_write  1 1 2000 rsq 0.01 2.5 lj1_lj2.table lj
```

Note that it is strongly recommended to try to **delete** the potential table file before generating it. Since the *pair_write* command will always **append** to a table file, while pair style table will use the **first match**. Thus when changing the potential function in the python class, the table pair style will still read the old variant unless the table file is first deleted.

After switching the pair style to *table*, the potential tables need to be assigned to the LAMMPS atom types like this:

```
pair_style      table linear 2000
pair_coeff      1  1  melt.table lj
```

This can also be done for more complex systems. Please see the *examples/python* folders for a few more examples.

Mixing, shift, table, tail correction, restart, rRESPA info:

Mixing of potential parameters has to be handled inside the provided python module. The python pair style simply assumes that force and energy computation can be correctly performed for all pairs of atom types as they are mapped to the atom type labels inside the python potential class.

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.373.4 Restrictions

This pair style is part of the PYTHON package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.373.5 Related commands

pair_coeff, *pair_write*, *pair style table*

Default: none

18.374 pair_style quip command

18.374.1 Syntax

```
pair_style quip
```

18.374.2 Examples

```
pair_style      quip
pair_coeff      * * gap_example.xml "Potential xml_label=GAP_2014_5_8_60_17_10_38_466
↪" 14
pair_coeff      * * sw_example.xml "IP SW" 14
```

18.374.3 Description

Style *quip* provides an interface for calling potential routines from the QUIP package. QUIP is built separately, and then linked to LAMMPS. The most recent version of the QUIP package can be downloaded from GitHub: https://github.com/libAtoms/QUIP. The interface is chiefly intended to be used to run Gaussian Approximation Potentials (GAP), which are described in the following publications: *(Bartok et al)* and *(PhD thesis of Bartok)*.

Only a single pair_coeff command is used with the *quip* style that specifies a QUIP potential file containing the parameters of the potential for all needed elements in XML format. This is followed by a QUIP initialization string. Finally, the QUIP elements are mapped to LAMMPS atom types by specifying N atomic numbers, where N is the number of LAMMPS atom types:

- QUIP filename
- QUIP initialization string
- N atomic numbers = mapping of QUIP elements to atom types

See the *pair_coeff* doc page for alternate ways to specify the path for the potential file.

A QUIP potential is fully specified by the filename which contains the parameters of the potential in XML format, the initialization string, and the map of atomic numbers.

GAP potentials can be obtained from the Data repository section of http://www.libatoms.org, where the appropriate initialization strings are also advised. The list of atomic numbers must be matched to the LAMMPS atom types specified in the LAMMPS data file or elsewhere.

Two examples input scripts are provided in the examples/USER/quip directory.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the *pair_modify* mix, shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.374.4 Restrictions

This pair style is part of the USER-QUIP package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

QUIP potentials are parameterized in electron-volts and Angstroms and therefore should be used with LAMMPS metal *units*.

QUIP potentials are generally not designed to work with the scaling factors set by the *special_bonds* command. The recommended setting in molecular systems is to include all interactions, i.e. to use *special_bonds lj/coul 1.0 1.0 1.0*. Scaling factors > 0.0 will be ignored and treated as 1.0. The only exception to this rule is if you know that your QUIP potential needs to exclude bonded, 1-3, or 1-4 interactions and does not already do this exclusion within QUIP. Then a

factor 0.0 needs to be used which will remove such pairs from the neighbor list. This needs to be very carefully tested, because it may remove pairs from the neighbor list that are still required.

18.374.5 Related commands

pair_coeff

(Bartok_2010) AP Bartok, MC Payne, R Kondor, and G Csanyi, Physical Review Letters 104, 136403 (2010).

(Bartok_PhD) A Bartok-Partay, PhD Thesis, University of Cambridge, (2010).

18.375 pair_style reax/c command

18.376 pair_style reax/c/kk command

18.377 pair_style reax/c/omp command

18.377.1 Syntax

```
pair_style reax/c cfile keyword value
```

- cfile = NULL or name of a control file
- zero or more keyword/value pairs may be appended

```
keyword = checkqeq or lgvdw or safezone or mincap
  checkqeq value = yes or no = whether or not to require qeq/reax fix
  enobonds value = yes or no = whether or not to tally energy of atoms␣
↪with no bonds
  lgvdw value = yes or no = whether or not to use a low gradient vdW␣
↪correction
  safezone = factor used for array allocation
  mincap = minimum size for array allocation
```

18.377.2 Examples

```
pair_style reax/c NULL
pair_style reax/c controlfile checkqeq no
pair_style reax/c NULL lgvdw yes
pair_style reax/c NULL safezone 1.6 mincap 100
pair_coeff * * ffield.reax C H O N
```

18.377.3 Description

Style *reax/c* computes the ReaxFF potential of van Duin, Goddard and co-workers. ReaxFF uses distance-dependent bond-order functions to represent the contributions of chemical bonding to the potential energy. There is more than one version of ReaxFF. The version implemented in LAMMPS uses the functional forms documented in the supplemental information of the following paper: *(Chenoweth et al., 2008)*. The version integrated into LAMMPS matches the most up-to-date version of ReaxFF as of summer 2010. For more technical details about the pair reax/c implementation of ReaxFF, see the *(Aktulga)* paper. The *reax/c* style was initially implemented as a stand-alone C code and is now integrated into LAMMPS as a package.

The *reax/c/kk* style is a Kokkos version of the ReaxFF potential that is derived from the *reax/c* style. The Kokkos version can run on GPUs and can also use OpenMP multithreading. For more information about the Kokkos package, see *Packages details* and *Speed kokkos* doc pages. One important consideration when using the *reax/c/kk* style is the choice of either half or full neighbor lists. This setting can be changed using the Kokkos *package* command.

The *reax/c* style differs from the (obsolete) "pair_style reax" command in the implementation details. The *reax* style was a Fortran library, linked to LAMMPS. The *reax* style has been removed from LAMMPS after the 12 December 2018 version.

LAMMPS provides several different versions of ffield.reax in its potentials dir, each called potentials/ffield.reax.label. These are documented in potentials/README.reax. The default ffield.reax contains parameterizations for the following elements: C, H, O, N.

The format of these files is identical to that used originally by van Duin. We have tested the accuracy of *pair_style reax/c* potential against the original ReaxFF code for the systems mentioned above. You can use other ffield files for specific chemical systems that may be available elsewhere (but note that their accuracy may not have been tested).

Note: We do not distribute a wide variety of ReaxFF force field files with LAMMPS. Adri van Duin's group at PSU is the central repository for this kind of data as they are continuously deriving and updating parameterizations for different classes of materials. You can submit a contact request at the Materials Computation Center (MCC) website https://www.mri.psu.edu/materials-computation-center/connect-mcc, describing the material(s) you are interested in modeling with ReaxFF. They can tell you what is currently available or what it would take to create a suitable ReaxFF parameterization.

The *cfile* setting can be specified as NULL, in which case default settings are used. A control file can be specified which defines values of control variables. Some control variables are global parameters for the ReaxFF potential. Others define certain performance and output settings. Each line in the control file specifies the value for a control variable. The format of the control file is described below.

Note: The LAMMPS default values for the ReaxFF global parameters correspond to those used by Adri van Duin's stand-alone serial code. If these are changed by setting control variables in the control file, the results from LAMMPS and the serial code will not agree.

Examples using *pair_style reax/c* are provided in the examples/reax sub-directory.

Use of this pair style requires that a charge be defined for every atom. See the *atom_style* and *read_data* commands for details on how to specify charges.

The ReaxFF parameter files provided were created using a charge equilibration (QEq) model for handling the electrostatic interactions. Therefore, by default, LAMMPS requires that the *fix qeq/reax* command be used with *pair_style reax/c* when simulating a ReaxFF model, to equilibrate charge each timestep. Using the keyword *checkqeq* with the value *no* turns off the check for *fix qeq/reax*, allowing a simulation to be run without charge equilibration. In this case, the static charges you assign to each atom will be used for computing the electrostatic interactions in the system. See the *fix qeq/reax* command for details.

Using the optional keyword *lgvdw* with the value *yes* turns on the low-gradient correction of the ReaxFF/C for long-range London Dispersion, as described in the *(Liu)* paper. Force field file *ffield.reax.lg* is designed for this correction, and is trained for several energetic materials (see "Liu"). When using lg-correction, recommended value for parameter *thb* is 0.01, which can be set in the control file. Note: Force field files are different for the original or lg corrected pair styles, using wrong ffield file generates an error message.

Using the optional keyword *enobonds* with the value *yes*, the energy of atoms with no bonds (i.e. isolated atoms) is included in the total potential energy and the per-atom energy of that atom. If the value *no* is specified then the energy of atoms with no bonds is set to zero. The latter behavior is usual not desired, as it causes discontinuities in the potential energy when the bonding of an atom drops to zero.

Optional keywords *safezone* and *mincap* are used for allocating reax/c arrays. Increasing these values can avoid memory problems, such as segmentation faults and bondchk failed errors, that could occur under certain conditions. These keywords aren't used by the Kokkos version, which instead uses a more robust memory allocation scheme that checks if the sizes of the arrays have been exceeded and automatically allocates more memory.

The thermo variable *evdwl* stores the sum of all the ReaxFF potential energy contributions, with the exception of the Coulombic and charge equilibration contributions which are stored in the thermo variable *ecoul*. The output of these quantities is controlled by the *thermo* command.

This pair style tallies a breakdown of the total ReaxFF potential energy into sub-categories, which can be accessed via the *compute pair* command as a vector of values of length 14. The 14 values correspond to the following sub-categories (the variable names in italics match those used in the original FORTRAN ReaxFF code):

1. *eb* = bond energy
2. *ea* = atom energy
3. *elp* = lone-pair energy
4. *emol* = molecule energy (always 0.0)
5. *ev* = valence angle energy
6. *epen* = double-bond valence angle penalty
7. *ecoa* = valence angle conjugation energy
8. *ehb* = hydrogen bond energy
9. *et* = torsion energy
10. *eco* = conjugation energy
11. *ew* = van der Waals energy
12. *ep* = Coulomb energy
13. *efi* = electric field energy (always 0.0)
14. *eqeq* = charge equilibration energy

To print these quantities to the log file (with descriptive column headings) the following commands could be included in an input script:

```
compute reax all pair reax/c
variable eb      equal c_reax[1]
variable ea      equal c_reax[2]
[...]
variable eqeq    equal c_reax[14]
thermo_style custom step temp epair v_eb v_ea [...] v_eqeq
```

Only a single pair_coeff command is used with the *reax/c* style which specifies a ReaxFF potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N indices = ReaxFF elements

The filename is the ReaxFF potential file.

In the ReaxFF potential file, near the top, after the general parameters, is the atomic parameters section that contains element names, each with a couple dozen numeric parameters. If there are M elements specified in the *ffield* file, think of these as numbered 1 to M. Each of the N indices you specify for the N atom types of LAMMPS atoms must be an integer from 1 to M. Atoms with LAMMPS type 1 will be mapped to whatever element you specify as the first index value, etc. If a mapping value is specified as NULL, the mapping is not performed. This can be used when the *reax/c* style is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

As an example, say your LAMMPS simulation has 4 atom types and the elements are ordered as C, H, O, N in the *ffield* file. If you want the LAMMPS atom type 1 and 2 to be C, type 3 to be N, and type 4 to be H, you would use the following pair_coeff command:

```
pair_coeff * * ffield.reax C C N H
```

The format of a line in the control file is as follows:

```
variable_name value
```

and it may be followed by an "!" character and a trailing comment.

If the value of a control variable is not specified, then default values are used. What follows is the list of variables along with a brief description of their use and default values.

simulation_name: Output files produced by *pair_style reax/c* carry this name + extensions specific to their contents. Partial energies are reported with a ".pot" extension, while the trajectory file has ".trj" extension.

tabulate_long_range: To improve performance, long range interactions can optionally be tabulated (0 means no tabulation). Value of this variable denotes the size of the long range interaction table. The range from 0 to long range cutoff (defined in the *ffield* file) is divided into *tabulate_long_range* points. Then at the start of simulation, we fill in the entries of the long range interaction table by computing the energies and forces resulting from van der Waals and Coulomb interactions between every possible atom type pairs present in the input system. During the simulation we consult to the long range interaction table to estimate the energy and forces between a pair of atoms. Linear interpolation is used for estimation. (default value = 0)

energy_update_freq: Denotes the frequency (in number of steps) of writes into the partial energies file. (default value = 0)

nbrhood_cutoff: Denotes the near neighbors cutoff (in Angstroms) regarding the bonded interactions. (default value = 5.0)

hbond_cutoff: Denotes the cutoff distance (in Angstroms) for hydrogen bond interactions.(default value = 7.5. A value of 0.0 turns off hydrogen bonds)

bond_graph_cutoff: is the threshold used in determining what is a physical bond, what is not. Bonds and angles reported in the trajectory file rely on this cutoff. (default value = 0.3)

thb_cutoff: cutoff value for the strength of bonds to be considered in three body interactions. (default value = 0.001)

thb_cutoff_sq: cutoff value for the strength of bond order products to be considered in three body interactions. (default value = 0.00001)

write_freq: Frequency of writes into the trajectory file. (default value = 0)

traj_title: Title of the trajectory - not the name of the trajectory file.

atom_info: 1 means print only atomic positions + charge (default = 0)

atom_forces: 1 adds net forces to atom lines in the trajectory file (default = 0)

atom_velocities: 1 adds atomic velocities to atoms line (default = 0)

bond_info: 1 prints bonds in the trajectory file (default = 0)

angle_info: 1 prints angles in the trajectory file (default = 0)

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the *pair_modify* mix, shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

18.377.4 Restrictions

This pair style is part of the USER-REAXC package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

The ReaxFF potential files provided with LAMMPS in the potentials directory are parameterized for real *units*. You can use the ReaxFF potential with any LAMMPS units, but you would need to create your own potential file with coefficients listed in the appropriate units if your simulation doesn't use "real" units.

18.377.5 Related commands

pair_coeff, *fix qeq/reax*, *fix reax/c/bonds*, *fix reax/c/species*

18.377.6 Default

The keyword defaults are checkqeq = yes, enobonds = yes, lgvdw = no, safezone = 1.2, mincap = 50.

(Chenoweth_2008) Chenoweth, van Duin and Goddard, Journal of Physical Chemistry A, 112, 1040-1053 (2008).

(Aktulga) Aktulga, Fogarty, Pandit, Grama, Parallel Computing, 38, 245-259 (2012).

(Liu) L. Liu, Y. Liu, S. V. Zybin, H. Sun and W. A. Goddard, Journal of Physical Chemistry A, 115, 11016-11022 (2011).

18.378 pair_style resquared command

18.379 pair_style resquared/gpu command

18.380 pair_style resquared/omp command

18.380.1 Syntax

```
pair_style resquared cutoff
```

- cutoff = global cutoff for interactions (distance units)

18.380.2 Examples

```
pair_style resquared 10.0
pair_coeff * * 1.0 1.0 1.7 3.4 3.4 1.0 1.0 1.0
```

18.380.3 Description

Style *resquared* computes the RE-squared anisotropic interaction *(Everaers)*, *(Babadi)* between pairs of ellipsoidal and/or spherical Lennard-Jones particles. For ellipsoidal interactions, the potential considers the ellipsoid as being comprised of small spheres of size σ. LJ particles are a single sphere of size σ. The distinction is made to allow the pair style to make efficient calculations of ellipsoid/solvent interactions.

Details for the equations used are given in the references below and in this supplementary document.

Use of this pair style requires the NVE, NVT, or NPT fixes with the *asphere* extension (e.g. *fix nve/asphere*) in order to integrate particle rotation. Additionally, *atom_style ellipsoid* should be used since it defines the rotational state and the size and shape of each ellipsoidal particle.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- A12 = Energy Prefactor/Hamaker constant (energy units)
- σ = atomic interaction diameter (distance units)
- $\epsilon_{i,a}$ = relative well depth of type I for side-to-side interactions
- $\epsilon_{i,b}$ = relative well depth of type I for face-to-face interactions

- $\epsilon_{i,c}$ = relative well depth of type I for end-to-end interactions
- $\epsilon_{j,a}$ = relative well depth of type J for side-to-side interactions
- $\epsilon_{j,b}$ = relative well depth of type J for face-to-face interactions
- $\epsilon_{j,c}$ = relative well depth of type J for end-to-end interactions
- cutoff (distance units)

The parameters used depend on the type of the interacting particles, i.e. ellipsoids or LJ spheres. The type of a particle is determined by the diameters specified for its 3 shape parameters. If all 3 shape parameters = 0.0, then the particle is treated as an LJ sphere. The $\epsilon_{i,*}$ or $\epsilon_{j,*}$ parameters are ignored for LJ spheres. If the 3 shape parameters are > 0.0, then the particle is treated as an ellipsoid (even if the 3 parameters are equal to each other).

A12 specifies the energy prefactor which depends on the types of the two interacting particles.

For ellipsoid/ellipsoid interactions, the interaction is computed by the formulas in the supplementary document referenced above. A12 is the Hamaker constant as described in *(Everaers)*. In LJ units:

$$A_{12} = 4\pi^2 \epsilon_{\mathrm{LJ}} (\rho\sigma^3)^2$$

where ρ gives the number density of the spherical particles composing the ellipsoids and ϵ_{LJ} determines the interaction strength of the spherical particles.

For ellipsoid/LJ sphere interactions, the interaction is also computed by the formulas in the supplementary document referenced above. A12 has a modified form (see here for details):

$$A_{12} = 4\pi^2 \epsilon_{\mathrm{LJ}} (\rho\sigma^3)$$

For ellipsoid/LJ sphere interactions, a correction to the distance- of-closest approach equation has been implemented to reduce the error from two particles of disparate sizes; see this supplementary document.

For LJ sphere/LJ sphere interactions, the interaction is computed using the standard Lennard-Jones formula, which is much cheaper to compute than the ellipsoidal formulas. A12 is used as epsilon in the standard LJ formula:

$$A_{12} = \epsilon_{\mathrm{LJ}}$$

and the specified σ is used as the σ in the standard LJ formula.

When one of both of the interacting particles are ellipsoids, then σ specifies the diameter of the continuous distribution of constituent particles within each ellipsoid used to model the RE-squared potential. Note that this is a different meaning for σ than the *pair_style gayberne* potential uses.

The ϵ_i and ϵ_j coefficients are defined for atom types, not for pairs of atom types. Thus, in a series of pair_coeff commands, they only need to be specified once for each atom type.

Specifically, if any of $\epsilon_{i,a}$, $\epsilon_{i,b}$, $\epsilon_{i,c}$ are non-zero, the three values are assigned to atom type I. If all the ϵ_i values are zero, they are ignored. If any of $\epsilon_{j,a}$, $\epsilon_{j,b}$, $\epsilon_{j,c}$ are non-zero, the three values are assigned to atom type J. If all three ϵ_i values are zero, they are ignored. Thus the typical way to define the ϵ_i and ϵ_j coefficients is to list their values in "pair_coeff I J" commands when I = J, but set them to 0.0 when I != J. If you do list them when I != J, you should insure they are consistent with their values in other pair_coeff commands.

Note that if this potential is being used as a sub-style of *pair_style hybrid*, and there is no "pair_coeff I I" setting made for RE-squared for a particular type I (because I-I interactions are computed by another hybrid pair potential), then you still need to insure the epsilon a,b,c coefficients are assigned to that type in a "pair_coeff I J" command.

For large uniform molecules it has been shown that the epsilon_*_* energy parameters are approximately representable in terms of local contact curvatures *(Everaers)*:

$$\epsilon_a = \sigma \cdot \frac{a}{b \cdot c}; \epsilon_b = \sigma \cdot \frac{b}{a \cdot c}; \epsilon_c = \sigma \cdot \frac{c}{a \cdot b}$$

where a, b, and c give the particle diameters.

The last coefficient is optional. If not specified, the global cutoff specified in the pair_style command is used.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance can be mixed, but only for sphere pairs. The default mix value is *geometric*. See the "pair_modify" command for details. Other type pairs cannot be mixed, due to the different meanings of the energy prefactors used to calculate the interactions and the implicit dependence of the ellipsoid-sphere interaction on the equation for the Hamaker constant presented here. Mixing of sigma and epsilon followed by calculation of the energy prefactors using the equations above is recommended.

This pair styles supports the *pair_modify* shift option for the energy of the Lennard-Jones portion of the pair interaction, but only for sphere-sphere interactions. There is no shifting performed for ellipsoidal interactions due to the anisotropic dependence of the interaction.

The *pair_modify* table option is not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords of the *run_style command*.

18.380.4 Restrictions

This style is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This pair style requires that atoms be ellipsoids as defined by the *atom_style ellipsoid* command.

Particles acted on by the potential can be finite-size aspherical or spherical particles, or point particles. Spherical particles have all 3 of their shape parameters equal to each other. Point particles have all 3 of their shape parameters equal to 0.0.

The distance-of-closest-approach approximation used by LAMMPS becomes less accurate when high-aspect ratio ellipsoids are used.

18.380.5 Related commands

pair_coeff, *fix nve/asphere*, *compute temp/asphere*, *pair_style gayberne*

Default: none

(Everaers) Everaers and Ejtehadi, Phys Rev E, 67, 041710 (2003).

(Berardi) Babadi, Ejtehadi, Everaers, J Comp Phys, 219, 770-779 (2006).

18.381 pair_style lj/sdk command

18.382 pair_style lj/sdk/gpu command

18.383 pair_style lj/sdk/kk command

18.384 pair_style lj/sdk/omp command

18.385 pair_style lj/sdk/coul/long command

18.386 pair_style lj/sdk/coul/long/gpu command

18.387 pair_style lj/sdk/coul/long/omp command

18.388 pair_style lj/sdk/coul/msm command

18.389 pair_style lj/sdk/coul/msm/omp command

18.389.1 Syntax

```
pair_style style args
```

- style = *lj/sdk* or *lj/sdk/coul/long*
- args = list of arguments for a particular style

```
lj/sdk args = cutoff
  cutoff = global cutoff for Lennard Jones interactions (distance units)
lj/sdk/coul/long args = cutoff (cutoff2)
  cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
  cutoff2 = global cutoff for Coulombic (optional) (distance units)
```

18.389.2 Examples

```
pair_style lj/sdk 2.5
pair_coeff 1 1 lj12_6 1 1.1 2.8

pair_style lj/sdk/coul/long 10.0
pair_style lj/sdk/coul/long 10.0 12.0
pair_coeff 1 1 lj9_6 100.0 3.5 12.0

pair_style lj/sdk/coul/msm 10.0
pair_style lj/sdk/coul/msm 10.0 12.0
pair_coeff 1 1 lj9_6 100.0 3.5 12.0
```

18.389.3 Description

The *lj/sdk* styles compute a 9/6, 12/4, or 12/6 Lennard-Jones potential, given by

$$E = \frac{27}{4}\epsilon\left[\left(\frac{\sigma}{r}\right)^9 - \left(\frac{\sigma}{r}\right)^6\right] \qquad r < r_c$$
$$E = \frac{3\sqrt{3}}{2}\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^4\right] \qquad r < r_c$$
$$E = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right] \qquad r < r_c$$

as required for the SDK Coarse-grained MD parameterization discussed in *(Shinoda)* and *(DeVane)*. Rc is the cutoff.

Style *lj/sdk/coul/long* computes the adds Coulombic interactions with an additional damping factor applied so it can be used in conjunction with the *kspace_style* command and its *ewald* or *pppm* or *pppm/cg* option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- cg_type (lj9_6, lj12_4, or lj12_6)
- epsilon (energy units)
- sigma (distance units)
- cutoff1 (distance units)

Note that sigma is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum. The prefactors are chosen so that the potential minimum is at -epsilon.

The latter 2 coefficients are optional. If not specified, the global LJ and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both LJ and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the LJ and Coulombic cutoffs for this type pair.

For *lj/sdk/coul/long* and *lj/sdk/coul/msm* only the LJ cutoff can be specified since a Coulombic cutoff cannot be specified for an individual I,J type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

Styles with a *gpu*, *intel*, *kk*, *omp* or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages*

doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP, and OPT packages respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, and rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/sdk pair styles *cannot* be mixed, since different pairs may have different exponents. So all parameters for all pairs have to be specified explicitly through the "pair_coeff" command. Defining then in a data file is also not supported, due to limitations of that file format.

All of the lj/sdk pair styles support the *pair_modify* shift option for the energy of the Lennard-Jones portion of the pair interaction.

The *lj/sdk/coul/long* pair styles support the *pair_modify* table option since they can tabulate the short-range portion of the long-range Coulombic interaction.

All of the lj/sdk pair styles write their information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

The lj/sdk and lj/cut/coul/long pair styles do not support the use of the *inner*, *middle*, and *outer* keywords of the *run_style respa* command.

18.389.4 Restrictions

All of the lj/sdk pair styles are part of the USER-CGSDK package. The *lj/sdk/coul/long* style also requires the KSPACE package to be built (which is enabled by default). They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.389.5 Related commands

pair_coeff, *angle_style sdk*

Default: none

(Shinoda) Shinoda, DeVane, Klein, Mol Sim, 33, 27 (2007).

(DeVane) Shinoda, DeVane, Klein, Soft Matter, 4, 2453-2462 (2008).

18.390 pair_style sdpd/taitwater/isothermal command

18.390.1 Syntax

```
pair_style sdpd/taitwater/isothermal temperature viscosity seed
```

- temperature = temperature of the fluid (temperature units)
- viscosity = dynamic viscosity of the fluid (mass*distance/time units)
- seed = random number generator seed (positive integer, optional)

18.390.2 Examples

```
pair_style sdpd/taitwater/isothermal 300. 1. 28681
pair_coeff * * 1000.0 1430.0 2.4
```

18.390.3 Description

The sdpd/taitwater/isothermal style computes forces between mesoscopic particles according to the Smoothed Dissipative Particle Dynamics model described in this paper by *(Espanol and Revenga)* under the following assumptions:

1. The temperature is constant and uniform.
2. The shear viscosity is constant and uniform.
3. The volume viscosity is negligible before the shear viscosity.
4. The Boltzmann constant is negligible before the heat capacity of a single mesoscopic particle of fluid.

The third assumption is true for water in nearly incompressible flows. The fourth holds true for water for any reasonable size one can imagine for a mesoscopic particle.

The pressure forces between particles will be computed according to Tait's equation of state:

$$p = B\left[(\frac{\rho}{\rho_0})^\gamma - 1\right]$$

where $\gamma = 7$ and $B = c_0^2\rho_0/\gamma$, with ρ_0 being the reference density and c_0 the reference speed of sound.

The laminar viscosity and the random forces will be computed according to formulas described in *(Espanol and Revenga)*.

Warning: Similar to *brownian* and *dpd* styles, the *newton* setting for pairwise interactions needs to be on when running LAMMPS in parallel if you want to ensure linear momentum conservation. Otherwise random forces generated for pairs straddling processor boundary will not be equal and opposite.

Note: The actual random seed used will be a mix of what you specify and other parameters like the MPI ranks. This is to ensure that different MPI tasks have distinct seeds.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above.

- ρ_0 reference density (mass/volume units)
- c_0 reference soundspeed (distance/time units)
- h kernel function cutoff (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the *pair_modify* shift, table, and tail options.

This style does not write information to *binary restart files*. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.390.4 Restrictions

This pair style is part of the USER-SDPD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.390.5 Related commands

pair coeff, *pair sph/rhosum*, *pair sph/taitwater*

18.390.6 Default

The default seed is 0 (before mixing).

(Espanol and Revenga) Espanol, Revenga, Physical Review E, 67, 026705 (2003).

18.391 pair_style smd/hertz command

18.391.1 Syntax

```
pair_style smd/hertz scale_factor
```

18.391.2 Examples

```
pair_style smd/hertz 1.0
pair_coeff 1 1 <contact_stiffness>
```

18.391.3 Description

The *smd/hertz* style calculates contact forces between SPH particles belonging to different physical bodies.

The contact forces are calculated using a Hertz potential, which evaluates the overlap between two particles (whose spatial extents are defined via its contact radius). The effect is that a particles cannot penetrate into each other. The parameter <contact_stiffness> has units of pressure and should equal roughly one half of the Young's modulus (or bulk modulus in the case of fluids) of the material model associated with the SPH particles.

The parameter *scale_factor* can be used to scale the particles' contact radii. This can be useful to control how close particles can approach each other. Usually, *scale_factor* =1.0.

Mixing, shift, table, tail correction, restart, rRESPA info:

No mixing is performed automatically. Currently, no part of USER-SMD supports restarting nor minimization. rRESPA does not apply to this pair style.

18.391.4 Restrictions

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.391.5 Related commands

pair_coeff

Default: none

18.392 pair_style smd/tlsph command

18.392.1 Syntax

```
pair_style smd/tlsph args
```

18.392.2 Examples

```
pair_style smd/tlsph
```

18.392.3 Description

The *smd/tlsph* style computes particle interactions according to continuum mechanics constitutive laws and a Total-Lagrangian Smooth-Particle Hydrodynamics algorithm.

This pair style is invoked with the following command:

```
pair_style smd/tlsph
pair_coeff i j *COMMON rho0 E nu Q1 Q2 hg Cp &
               *END
```

Here, *i* and *j* denote the *LAMMPS* particle types for which this pair style is defined. Note that *i* and *j* must be equal, i.e., no *tlsph* cross interactions between different particle types are allowed. In contrast to the usual *LAMMPS pair coeff* definitions, which are given solely a number of floats and integers, the *tlsph pair coeff* definition is organized using keywords. These keywords mark the beginning of different sets of parameters for particle properties, material constitutive models, and damage models. The *pair coeff* line must be terminated with the **END* keyword. The use the line continuation operator *&* is recommended. A typical invocation of the *tlsph* for a solid body would consist of an equation of state for computing the pressure (the diagonal components of the stress tensor), and a material model to compute shear stresses (the off-diagonal components of the stress tensor). Damage and failure models can also be added.

Please see the SMD user guide for a complete listing of the possible keywords and material models.

Mixing, shift, table, tail correction, restart, rRESPA info:

No mixing is performed automatically. Currently, no part of USER-SMD supports restarting nor minimization. rRESPA does not apply to this pair style.

18.392.4 Restrictions

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.392.5 Related commands

pair_coeff

Default: none

18.393 pair_style smd/tri_surface command

18.393.1 Syntax

```
pair_style smd/tri_surface scale_factor
```

18.393.2 Examples

```
pair_style smd/tri_surface 1.0
pair_coeff 1 1 <contact_stiffness>
```

18.393.3 Description

The *smd/tri_surface* style calculates contact forces between SPH particles and a rigid wall boundary defined via the *smd/wall_surface* fix.

The contact forces are calculated using a Hertz potential, which evaluates the overlap between a particle (whose spatial extents are defined via its contact radius) and the triangle. The effect is that a particle cannot penetrate into the triangular surface. The parameter <contact_stiffness> has units of pressure and should equal roughly one half of the Young's modulus (or bulk modulus in the case of fluids) of the material model associated with the SPH particle

The parameter *scale_factor* can be used to scale the particles' contact radii. This can be useful to control how close particles can approach the triangulated surface. Usually, *scale_factor* =1.0.

Mixing, shift, table, tail correction, restart, rRESPA info:

No mixing is performed automatically. Currently, no part of USER-SMD supports restarting nor minimization. rRESPA does not apply to this pair style.

18.393.4 Restrictions

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.393.5 Related commands

pair_coeff

Default: none

18.394 pair_style smd/ulsph command

18.394.1 Syntax

```
pair_style smd/ulsph args
```

- these keywords must be given

```
keyword = *DENSITY_SUMMATION or *DENSITY_CONTINUITY and *VELOCITY_GRADIENT␣
↪or *NO_VELOCITY_GRADIENT and *GRADIENT_CORRECTION or *NO_GRADIENT_
↪CORRECTION
```

18.394.2 Examples

```
pair_style smd/ulsph *DENSITY_CONTINUITY *VELOCITY_GRADIENT *NO_GRADIENT_CORRECTION
```

18.394.3 Description

The *smd/ulsph* style computes particle interactions according to continuum mechanics constitutive laws and an updated Lagrangian Smooth-Particle Hydrodynamics algorithm.

This pair style is invoked similar to the following command:

```
pair_style smd/ulsph *DENSITY_CONTINUITY *VELOCITY_GRADIENT *NO_GRADIENT_CORRECTION
pair_coeff i j *COMMON rho0 c0 Q1 Cp hg &
               *END
```

Here, *i* and *j* denote the *LAMMPS* particle types for which this pair style is defined. Note that *i* and *j* can be different, i.e., *ulsph* cross interactions between different particle types are allowed. However, *i–i* respectively *j–j* pair_coeff lines have to precede a cross interaction. In contrast to the usual *LAMMPS pair coeff* definitions, which are given solely a number of floats and integers, the *ulsph pair coeff* definition is organized using keywords. These keywords mark the beginning of different sets of parameters for particle properties, material constitutive models, and damage models. The *pair coeff* line must be terminated with the **END* keyword. The use the line continuation operator *&* is recommended. A typical invocation of the *ulsph* for a solid body would consist of an equation of state for computing the pressure (the diagonal components of the stress tensor), and a material model to compute shear stresses (the off-diagonal components of the stress tensor).

Note that the use of *GRADIENT_CORRECTION can lead to severe numerical instabilities. For a general fluid simulation, *NO_GRADIENT_CORRECTION is recommended.

Please see the SMD user guide for a complete listing of the possible keywords and material models.

Mixing, shift, table, tail correction, restart, rRESPA info:

No mixing is performed automatically. Currently, no part of USER-SMD supports restarting nor minimization. rRESPA does not apply to this pair style.

18.394.4 Restrictions

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.394.5 Related commands

pair_coeff

Default: none

18.395 pair_style smtbq command

18.395.1 Syntax

```
pair_style smtbq
```

18.395.2 Examples

```
pair_style smtbq
pair_coeff * * ffield.smtbq.Al2O3 O Al
```

18.395.3 Description

This pair style computes a variable charge SMTB-Q (Second-Moment tight-Binding QEq) potential as described in *SMTB-Q_1* and *SMTB-Q_2*. Briefly, the energy of metallic-oxygen systems is given by three contributions:

$$
\begin{aligned}
E_{tot} &= E_{ES} + E_{OO} + E_{MO} \\
E_{ES} &= \sum_i \left[\chi_i^0 Q_i + \frac{1}{2} J_i^0 Q_i^2 + \frac{1}{2} \sum_{j \neq i} J_{ij}(r_{ij}) f_{cut}^{R_{coul}}(r_{ij}) Q_i Q_j \right] \\
E_{OO} &= \sum_{i,j}^{i,j=O} \left[C exp(-\frac{r_{ij}}{\rho}) - D f_{cut}^{r_1^{OO} r_2^{OO}}(r_{ij}) exp(B r_{ij}) \right] \\
E_{MO} &= \sum_i E_{cov}^i + \sum_{j \neq i} A f_{cut}^{r_{c1} r_{c2}}(r_{ij}) exp\left[-p(\frac{r_{ij}}{r_0} - 1)\right]
\end{aligned}
$$

where E_{tot} is the total potential energy of the system, E_{ES} is the electrostatic part of the total energy, E_{OO} is the interaction between oxygen atoms and E_{MO} is a short-range interaction between metal and oxygen atoms. This interactions depend on interatomic distance r_{ij} and/or the charge Q_i of atoms *i*. Cut-off function enables smooth convergence to zero interaction.

The parameters appearing in the upper expressions are set in the ffield.SMTBQ.Syst file where Syst corresponds to the selected system (e.g. field.SMTBQ.Al2O3). Examples for TiO_2, Al_2O_3 are provided. A single pair_coeff command is used with the SMTBQ styles which provides the path to the potential file with parameters for needed elements. These are mapped to LAMMPS atom types by specifying additional arguments after the potential filename in the pair_coeff command. Note that atom type 1 must always correspond to oxygen atoms. As an example, to simulate a TiO_2 system, atom type 1 has to be oxygen and atom type 2 Ti. The following pair_coeff command should then be used:

```
pair_coeff * * PathToLammps/potentials/ffield.smtbq.TiO2 O Ti
```

The electrostatic part of the energy consists of two components

self-energy of atom *i* in the form of a second order charge dependent polynomial and a long-range Coulombic electrostatic interaction. The latter uses the wolf summation method described in *Wolf*, spherically truncated at a longer cutoff, R_{coul}. The charge of each ion is modeled by an orbital Slater which depends on the principal quantum number (*n*) of the outer orbital shared by the ion.

Interaction between oxygen, E_{OO}, consists of two parts, an attractive and a repulsive part. The attractive part is effective only at short range (< r_2^{OO}). The attractive contribution was optimized to study surfaces reconstruction (e.g. *SMTB-Q_2* in TiO_2) and is not necessary for oxide bulk modeling. The repulsive part is the Pauli interaction between the electron clouds of oxygen. The Pauli repulsion and the coulombic electrostatic interaction have same cut off value.

In the ffield.SMTBQ.Syst, the keyword *'buck'* allows to consider only the repulsive O-O interactions. The keyword *'buckPlusAttr'* allows to consider the repulsive and the attractive O-O interactions.

The short-range interaction between metal-oxygen, E_{MO} is based on the second moment approximation of the density of states with a N-body potential for the band energy term, E^i_{cov}, and a Born-Mayer type repulsive terms as indicated by the keyword *'second_moment'* in the ffield.SMTBQ.Syst. The energy band term is given by:

$$E^{i(i=M,O)}_{cov} = -\left\{\eta_i(\mu\xi^0)^2 f^{r_{c1}r_{c2}}_{cut}(r_{ij})\left(\sum_{j(j=O,M)} exp[-2q(\frac{r_{ij}}{r_0}-1)]\right)\delta Q_i\big(2\frac{n_0}{\eta_i}-\delta Q_i\big)\right\}^{1/2}$$

$$\delta Q_i = |Q^F_i| - |Q_i|$$

where η_i is the stoichiometry of atom *i*, δQ_i is the charge delocalization of atom *i*, compared to its formal charge Q^F_i. n_0, the number of hybridized orbitals, is calculated with to the atomic orbitals shared d_i and the stoichiometry η_i. r_{c1} and r_{c2} are the two cutoff radius around the fourth neighbors in the cutoff function.

In the formalism used here, ξ^0 is the energy parameter. ξ^0 is in tight-binding approximation the hopping integral between the hybridized orbitals of the cation and the anion. In the literature we find many ways to write the hopping integral depending on whether one takes the point of view of the anion or cation. These are equivalent vision. The correspondence between the two visions is explained in appendix A of the article in the SrTiO3 *SMTB-Q_3* (parameter β shown in this article is in fact the β_O). To summarize the relationship between the hopping integral ξ^O and the others, we have in an oxide $\mathrm{C_nO_m}$ the following relationship:

$$\xi^0 = \frac{\xi_O}{m} = \frac{\xi_C}{n}$$

$$\frac{\beta_O}{\sqrt{m}} = \frac{\beta_C}{\sqrt{n}} = \xi^0\frac{\sqrt{m}+\sqrt{n}}{2}$$

Thus parameter μ, indicated above, is given by $\mu = \frac{1}{2}(\sqrt{n}+\sqrt{m})$

The potential offers the possibility to consider the polarizability of the electron clouds of oxygen by changing the slater radius of the charge density around the oxygen atoms through the parameters *rBB, rB and rS* in the ffield.SMTBQ.Syst. This change in radius is performed according to the method developed by E. Maras *SMTB-Q_2*. This method needs to determine the number of nearest neighbors around the oxygen. This calculation is based on first (r_{1n}) and second (r_{2n}) distances neighbors.

The SMTB-Q potential is a variable charge potential. The equilibrium charge on each atom is calculated by the electronegativity equalization (QEq) method. See *Rick* for further detail. One can adjust the frequency, the maximum number of iterative loop and the convergence of the equilibrium charge calculation. To obtain the energy conservation in NVE thermodynamic ensemble, we recommend to use a convergence parameter in the interval 10e-5 - 10e-6 eV.

The ffield.SMTBQ.Syst files are provided for few systems. They consist of nine parts and the lines beginning with '#' are comments (note that the number of comment lines matter). The first sections are on the potential parameters and others are on the simulation options and might be modified. Keywords are character type and must be enclosed in quotation marks (‘’).

1) Number of different element in the oxide:

- N_elem= 2 or 3
- Divider line

2) Atomic parameters

For the anion (oxygen)

- Name of element (char) and stoichiometry in oxide
- Formal charge and mass of element
- Principal quantum number of outer orbital n), electronegativity (χ^0_i) and hardness (J^0_i)

- Ionic radius parameters : max coordination number (*coordBB* = 6 by default), bulk coordination number *(coordB)*, surface coordination number *(coordS)* and *rBB, rB and rS* the slater radius for each coordination number. (**note : If you don't want to change the slater radius, use three identical radius values**)
- Number of orbital shared by the element in the oxide (d_i)
- Divider line

For each cations (metal):

- Name of element (char) and stoichiometry in oxide
- Formal charge and mass of element
- Number of electron in outer orbital *(ne)*, electronegativity (χ_i^0), hardness (J_i^0) and r_{Slater} the slater radius for the cation.
- Number of orbitals shared by the elements in the oxide (d_i)
- Divider line

3) Potential parameters:

- Keyword for element1, element2 and interaction potential ('second_moment' or 'buck' or 'buckPlusAttr') between element 1 and 2. If the potential is 'second_moment', specify 'oxide' or 'metal' for metal-oxygen or metal-metal interactions respectively.
- Potential parameter:
  - If type of potential is 'second_moment' : A (eV), *p*, ζ^0 (eV) and *q*, $r_{c1}(\mathrm{\AA})$, $r_{c2}(\mathrm{\AA})$ and $r_0(\mathrm{\AA})$
  - If type of potential is 'buck' : *C* (eV) and $\rho(\mathrm{\AA})$
  - If type of potential is 'buckPlusAttr' : *C* (eV) and $\rho(\mathrm{\AA})$ *D* (eV), *B* ($\mathrm{\AA}^{-1}$), $r_1^{OO}(\mathrm{\AA})$ and $r_2^{OO}(\mathrm{\AA})$
- Divider line

4) Tables parameters:

- Cutoff radius for the Coulomb interaction (R_{coul})
- Starting radius ($r_{min} = 1,18845\mathrm{\AA}$) and increments ($dr = 0.001\mathrm{\AA}$) for creating the potential table.
- Divider line

5) Rick model parameter:

- *Nevery* : parameter to set the frequency of the charge resolution. The charges are evaluated each *Nevery* time steps.
- Max number of iterative loop (*loopmax*) and convergence criterion (*prec*) in eV of the charge resolution
- Divider line

6) Coordination parameter:

- First (r_{1n}) and second (r_{2n}) neighbor distances in angstrom
- Divider line

7) Charge initialization mode:

- Keyword (*QInitMode*) and initial oxygen charge (Q_{init}). If keyword = 'true', all oxygen charges are initially set equal to Q_{init}. The charges on the cations are initially set in order to respect the neutrality of the box. If keyword = 'false', all atom charges are initially set equal to 0 if you use the *create_atoms* command or the charge specified in the file structure using *read_data* command.
- Divider line

8) Mode for the electronegativity equalization (Qeq)

- Keyword (*mode*) followed by:
  - QEqAll (one QEq group) | no parameters
  - QEqAllParallel (several QEq groups) | no parameters
  - Surface | zlim (QEq only for z>zlim)
- Parameter if necessary
- Divider line

9) Verbose

- If you want the code to work in verbose mode or not : 'true' or 'false'
- If you want to print or not in the file 'Energy_component.txt' the three main contributions to the energy of the system according to the description presented above : 'true' or 'false' and N_{Energy}. This option writes to the file every N_{Energy} time steps. If the value is 'false' then $N_{Energy} = 0$. The file takes into account the possibility to have several QEq groups *g* then it writes: time step, number of atoms in group *g*, electrostatic part of energy, E_{ES}, the interaction between oxygen, E_{OO}, and short range metal-oxygen interaction, E_{MO}.
- If you want to print to the file 'Electroneg_component.txt' the electronegativity component ($\frac{\partial E_{tot}}{\partial Q_i}$) or not: 'true' or 'false' and $N_{Electroneg}$. This option writes to the file every $N_{Electroneg}$ time steps. If the value is 'false' then $N_{Electroneg} = 0$. The file consist of atom number *i*, atom type (1 for oxygen and # higher than 1 for metal), atom position: *x*, *y* and *z*, atomic charge of atom *i*, electrostatic part of atom *i* electronegativity, covalent part of atom *i* electronegativity, the hopping integral of atom *i* $(Z\beta^2)_i$ and box electronegativity.

Note: This last option slows down the calculation dramatically. Use only with a single processor simulation.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the *pair_modify* mix, shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in potential files. Thus, you needs to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

Restriction:

This pair style is part of the USER-SMTBQ package and is only enabled if LAMMPS is built with that package. See the *Build package* doc page for more info.

This potential requires using atom type 1 for oxygen and atom type higher than 1 for metal atoms.

This pair style requires the *newton* setting to be "on" for pair interactions.

The SMTB-Q potential files provided with LAMMPS (see the potentials directory) are parameterized for metal *units*.

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(SMTB-Q_3) R. Tetot, N. Salles, S. Landron, E. Amzallag, Surface Science 616, 19-8722 28 (2013)

(Wolf) D. Wolf, P. Keblinski, S. R. Phillpot, J. Eggebrecht, J Chem Phys, 110, 8254 (1999).

(Rick) S. W. Rick, S. J. Stuart, B. J. Berne, J Chem Phys 101, 6141 (1994).

18.396 pair_style snap command

18.397 pair_style snap/kk command

18.397.1 Syntax

```
pair_style snap
```

18.397.2 Examples

```
pair_style snap
pair_coeff * * InP.snapcoeff InP.snapparam In In P P
```

18.397.3 Description

Pair style *snap* computes interactions using the spectral neighbor analysis potential (SNAP) *(Thompson)*. Like the GAP framework of Bartok et al. *(Bartok2010)*, *(Bartok2013)* which uses bispectrum components to characterize the local neighborhood of each atom in a very general way. The mathematical definition of the bispectrum calculation used by SNAP is identical to that used by *compute sna/atom*. In SNAP, the total energy is decomposed into a sum over atom energies. The energy of atom *i* is expressed as a weighted sum over bispectrum components.

$$E^i_{SNAP}(B^i_1, ..., B^i_K) = \beta^{\alpha_i}_0 + \sum_{k=1}^{K} \beta^{\alpha_i}_k B^i_k$$

where B^i_k is the *k*-th bispectrum component of atom *i*, and $\beta^{\alpha_i}_k$ is the corresponding linear coefficient that depends on :math:alpha_i`, the SNAP element of atom *i*. The number of bispectrum components used and their definitions depend on the value of *twojmax* defined in the SNAP parameter file described below. The bispectrum calculation is described in more detail in *compute sna/atom*.

Note that unlike for other potentials, cutoffs for SNAP potentials are not set in the pair_style or pair_coeff command; they are specified in the SNAP potential files themselves.

Only a single pair_coeff command is used with the *snap* style which specifies a SNAP coefficient file followed by a SNAP parameter file and then N additional arguments specifying the mapping of SNAP elements to LAMMPS atom types, where N is the number of LAMMPS atom types:

- SNAP coefficient file
- SNAP parameter file
- N element names = mapping of SNAP elements to atom types

As an example, if a LAMMPS indium phosphide simulation has 4 atoms types, with the first two being indium and the 3rd and 4th being phophorous, the pair_coeff command would look like this:

```
pair_coeff * * snap InP.snapcoeff InP.snapparam In In P P
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The two filenames are for the coefficient and parameter files, respectively. The two trailing 'In' arguments map LAMMPS atom types 1 and 2 to the SNAP 'In' element. The two trailing 'P' arguments map LAMMPS atom types 3 and 4 to the SNAP 'P' element.

If a SNAP mapping value is specified as NULL, the mapping is not performed. This can be used when a *snap* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

The name of the SNAP coefficient file usually ends in the ".snapcoeff" extension. It may contain coefficients for many SNAP elements. The only requirement is that it contain at least those element names appearing in the LAMMPS mapping list. The name of the SNAP parameter file usually ends in the ".snapparam" extension. It contains a small number of parameters that define the overall form of the SNAP potential. See the *pair_coeff* doc page for alternate ways to specify the path for these files.

Quite commonly, SNAP potentials are combined with one or more other LAMMPS pair styles using the *hybrid/overlay* pair style. As an example, the SNAP tantalum potential provided in the LAMMPS potentials directory combines the *snap* and *zbl* pair styles. It is invoked by the following commands:

```
variable zblcutinner equal 4
variable zblcutouter equal 4.8
variable zblz equal 73
pair_style hybrid/overlay &
zbl ${zblcutinner} ${zblcutouter} snap
pair_coeff * * zbl 0.0
pair_coeff 1 1 zbl ${zblz}
pair_coeff * * snap Ta06A.snapcoeff Ta06A.snapparam Ta
```

It is convenient to keep these commands in a separate file that can be inserted in any LAMMPS input script using the *include* command.

The top of the SNAP coefficient file can contain any number of blank and comment lines (start with #), but follows a strict format after that. The first non-blank non-comment line must contain two integers:

- nelem = Number of elements
- ncoeff = Number of coefficients

This is followed by one block for each of the *nelem* elements. The first line of each block contains three entries:

- Element symbol (text string)
- R = Element radius (distance units)
- w = Element weight (dimensionless)

This line is followed by *ncoeff* coefficients, one per line.

The SNAP parameter file can contain blank and comment lines (start with #) anywhere. Each non-blank non-comment line must contain one keyword/value pair. The required keywords are *rcutfac* and *twojmax*. Optional keywords are *rfac0*, *rmin0*, *switchflag*, *bzeroflag*, and *chunksize*.

The default values for these keywords are

- *rfac0* = 0.99363
- *rmin0* = 0.0
- *switchflag* = 0

- *bzeroflag* = 1
- *quadraticflag* = 1
- *chunksize* = 2000

The keyword *chunksize* is only applicable when using the pair style *snap* with the KOKKOS package and is ignored otherwise. This keyword controls the number of atoms in each pass used to compute the bispectrum components and is used to avoid running out of memory. For example if there are 4000 atoms in the simulation and the *chunksize* is set to 2000, the bispectrum calculation will be broken up into two passes.

Detailed definitions for all the other keywords are given on the *compute sna/atom* doc page.

If *quadraticflag* is set to 1, then the SNAP energy expression includes the quadratic term, 0.5*B^t.alpha.B, where alpha is a symmetric K by K matrix. The SNAP element file should contain $K(K+1)/2$ additional coefficients for each element, the upper-triangular elements of alpha.

Note: The previously used *diagonalstyle* keyword was removed in 2019, since all known SNAP potentials use the default value of 3.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS with user-specifiable parameters as described above. You never need to specify a pair_coeff command with I != J arguments for this style.

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

18.397.4 Restrictions

This style is part of the SNAP package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.397.5 Related commands

compute sna/atom, *compute snad/atom*, *compute snav/atom*

Default: none

(Thompson) Thompson, Swiler, Trott, Foiles, Tucker, J Comp Phys, 285, 316 (2015).

(Bartok2010) Bartok, Payne, Risi, Csanyi, Phys Rev Lett, 104, 136403 (2010).

(Bartok2013) Bartok, Gillan, Manby, Csanyi, Phys Rev B 87, 184115 (2013).

18.398 pair_style soft command

18.399 pair_style soft/gpu command

18.400 pair_style soft/omp command

18.400.1 Syntax

```
pair_style soft cutoff
```

- cutoff = global cutoff for soft interactions (distance units)

18.400.2 Examples

```
pair_style soft 1.0
pair_coeff * * 10.0
pair_coeff 1 1 10.0 3.0

pair_style soft 1.0
pair_coeff * * 0.0
variable prefactor equal ramp(0,30)
fix 1 all adapt 1 pair soft a * * v_prefactor
```

18.400.3 Description

Style *soft* computes pairwise interactions with the formula

$$E = A \left[1 + \cos \left(\frac{\pi r}{r_c} \right) \right] \qquad r < r_c$$

It is useful for pushing apart overlapping atoms, since it does not blow up as r goes to 0. A is a pre-factor that can be made to vary in time from the start to the end of the run (see discussion below), e.g. to start with a very soft potential and slowly harden the interactions over time. Rc is the cutoff. See the *fix nve/limit* command for another way to push apart overlapping atoms.

The following coefficients must be defined for each pair of atom types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- A (energy units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global soft cutoff is used.

Note: The syntax for *pair_coeff* with a single A coeff is different in the current version of LAMMPS than in older versions which took two values, Astart and Astop, to ramp between them. This functionality is now available in a more general form through the *fix adapt* command, as explained below. Note that if you use an old input script and specify Astart and Astop without a cutoff, then LAMMPS will interpret that as A and a cutoff, which is probably not what you want.

The *fix adapt* command can be used to vary A for one or more pair types over the course of a simulation, in which case pair_coeff settings for A must still be specified, but will be overridden. For example these commands will vary the prefactor A for all pairwise interactions from 0.0 at the beginning to 30.0 at the end of a run:

```
variable prefactor equal ramp(0,30)
fix 1 all adapt 1 pair soft a * * v_prefactor
```

Note that a formula defined by an *equal-style variable* can use the current timestep, elapsed time in the current run, elapsed time since the beginning of a series of runs, as well as access other variables.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the A coefficient and cutoff distance for this pair style can be mixed. A is always mixed via a *geometric* rule. The cutoff is mixed according to the pair_modify mix value. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style does not support the *pair_modify* shift option, since the pair interaction goes to 0.0 at the cutoff.

The *pair_modify* table and tail options are not relevant for this pair style.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.400.4 Restrictions

none

18.400.5 Related commands

pair_coeff, *fix nve/limit*, *fix adapt*

Default: none

18.401 pair_style sph/heatconduction command

18.401.1 Syntax

```
pair_style sph/heatconduction
```

18.401.2 Examples

```
pair_style sph/heatconduction
pair_coeff * * 1.0 2.4
```

18.401.3 Description

The sph/heatconduction style computes heat transport between SPH particles. The transport model is the diffusion equation for the internal energy.

See this PDF guide to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above.

- D diffusion coefficient (length^2/time units)
- h kernel function cutoff (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the *pair_modify* shift, table, and tail options.

This style does not write information to *binary restart files*. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.401.4 Restrictions

This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.401.5 Related commands

pair_coeff, pair_sph/rhosum

Default: none

18.402 pair_style sph/idealgas command

18.402.1 Syntax

```
pair_style sph/idealgas
```

18.402.2 Examples

```
pair_style sph/idealgas
pair_coeff * * 1.0 2.4
```

18.402.3 Description

The sph/idealgas style computes pressure forces between particles according to the ideal gas equation of state:

$$p = (\gamma - 1)\rho e$$

where $\gamma = 1.4$ is the heat capacity ratio, ρ is the local density, and e is the internal energy per unit mass. This pair style also computes Monaghan's artificial viscosity to prevent particles from interpenetrating *(Monaghan)*.

See this PDF guide to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above.

- ν artificial viscosity (no units)
- h kernel function cutoff (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the *pair_modify* shift, table, and tail options.

This style does not write information to *binary restart files*. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.402.4 Restrictions

This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.402.5 Related commands

pair_coeff, pair_sph/rhosum

Default: none

(Monaghan) Monaghan and Gingold, Journal of Computational Physics, 52, 374-389 (1983).

18.403 pair_style sph/lj command

18.403.1 Syntax

```
pair_style sph/lj
```

18.403.2 Examples

```
pair_style sph/lj
pair_coeff * * 1.0 2.4
```

18.403.3 Description

The sph/lj style computes pressure forces between particles according to the Lennard-Jones equation of state, which is computed according to Ree's 1980 polynomial fit *(Ree)*. The Lennard-Jones parameters epsilon and sigma are set to unity. This pair style also computes Monaghan's artificial viscosity to prevent particles from interpenetrating *(Monaghan)*.

See this PDF guide to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above.

- ν artificial viscosity (no units)
- h kernel function cutoff (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the *pair_modify* shift, table, and tail options.

This style does not write information to *binary restart files*. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.403.4 Restrictions

As noted above, the Lennard-Jones parameters epsilon and sigma are set to unity.

This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.403.5 Related commands

pair_coeff, pair_sph/rhosum

Default: none

(Ree) Ree, Journal of Chemical Physics, 73, 5401 (1980).

(Monaghan) Monaghan and Gingold, Journal of Computational Physics, 52, 374-389 (1983).

18.404 pair_style sph/rhosum command

18.404.1 Syntax

```
pair_style sph/rhosum Nstep
```

- Nstep = timestep interval

18.404.2 Examples

```
pair_style sph/rhosum 10
pair_coeff * * 2.4
```

18.404.3 Description

The sph/rhosum style computes the local particle mass density rho for SPH particles by kernel function interpolation, every Nstep timesteps.

See this PDF guide to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above.

- h (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the *pair_modify* shift, table, and tail options.

This style does not write information to *binary restart files*. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.404.4 Restrictions

This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.404.5 Related commands

pair_coeff, pair_sph/taitwater

Default: none

18.405 pair_style sph/taitwater command

18.405.1 Syntax

```
pair_style sph/taitwater
```

18.405.2 Examples

```
pair_style sph/taitwater
pair_coeff * * 1000.0 1430.0 1.0 2.4
```

18.405.3 Description

The sph/taitwater style computes pressure forces between SPH particles according to Tait's equation of state:

$$p = B\left[\left(\frac{\rho}{\rho_0}\right)^{\gamma} - 1\right]$$

where $\gamma = 7$ and $B = c_0^2\rho_0/\gamma$, with ρ_0 being the reference density and c_0 the reference speed of sound.

This pair style also computes Monaghan's artificial viscosity to prevent particles from interpenetrating *(Monaghan)*.

See this PDF guide to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above.

- ρ_0 reference density (mass/volume units)
- c_0 reference soundspeed (distance/time units)
- ν artificial viscosity (no units)
- h kernel function cutoff (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the *pair_modify* shift, table, and tail options.

This style does not write information to *binary restart files*. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.405.4 Restrictions

This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.405.5 Related commands

pair_coeff, pair_sph/rhosum

Default: none

(Monaghan) Monaghan and Gingold, Journal of Computational Physics, 52, 374-389 (1983).

18.406 pair_style sph/taitwater/morris command

18.406.1 Syntax

```
pair_style sph/taitwater/morris
```

18.406.2 Examples

```
pair_style sph/taitwater/morris
pair_coeff * * 1000.0 1430.0 1.0 2.4
```

18.406.3 Description

The sph/taitwater/morris style computes pressure forces between SPH particles according to Tait's equation of state:

$$p = B\left[\left(\frac{\rho}{\rho_0}\right)^{\gamma} - 1\right]$$

where $\gamma = 7$ and $B = c_0^2\rho_0/\gamma$, with ρ_0 being the reference density and c_0 the reference speed of sound.

This pair style also computes laminar viscosity *(Morris)*.

See this PDF guide to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above.

- ρ_0 reference density (mass/volume units)
- c_0 reference soundspeed (distance/time units)
- ν dynamic viscosity (mass*distance/time units)
- h kernel function cutoff (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the *pair_modify* shift, table, and tail options.

This style does not write information to *binary restart files*. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.406.4 Restrictions

This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.406.5 Related commands

pair_coeff, pair_sph/rhosum

Default: none

(Morris) Morris, Fox, Zhu, J Comp Physics, 136, 214-226 (1997).

18.407 pair_style spin/dipole/cut command

18.408 pair_style spin/dipole/long command

18.408.1 Syntax

```
pair_style spin/dipole/cut cutoff
pair_style spin/dipole/long cutoff
```

- cutoff = global cutoff for magnetic dipole energy and forces (optional) (distance units)

18.408.2 Examples

```
pair_style spin/dipole/cut 10.0
pair_coeff * * 10.0
pair_coeff 2 3 8.0

pair_style spin/dipole/long 9.0
pair_coeff * * 10.0
pair_coeff 2 3 6.0
```

18.408.3 Description

Style *spin/dipole/cut* computes a short-range dipole-dipole interaction between pairs of magnetic particles that each have a magnetic spin. The magnetic dipole-dipole interactions are computed by the following formulas for the magnetic energy, magnetic precession vector omega and mechanical force between particles I and J.

$$\mathcal{H}_{\text{long}} = -\frac{\mu_0\,(\mu_B)^2}{4\pi}\sum_{i,j,i\neq j}^{N}\frac{g_i g_j}{r_{ij}^3}\left(3\,(\vec{e}_{ij}\cdot\vec{s}_i)\,(\vec{e}_{ij}\cdot\vec{s}_j)-\vec{s}_i\cdot\vec{s}_j\right)$$

$$\omega_i = \frac{\mu_0(\mu_B)^2}{4\pi\hbar}\sum_j\frac{g_i g_j}{r_{ij}^3}\left(3\,(\vec{e}_{ij}\cdot\vec{s}_j)\vec{e}_{ij}-\vec{s}_j\right)$$

$$\mathbf{F}_i = \frac{3\,\mu_0(\mu_B)^2}{4\pi}\sum_j\frac{g_i g_j}{r_{ij}^4}\left[\big((\vec{s}_i\cdot\vec{s}_j)-5(\vec{e}_{ij}\cdot\vec{s}_i)(\vec{e}_{ij}\cdot\vec{s}_j)\big)\vec{e}_{ij}+\big((\vec{e}_{ij}\cdot\vec{s}_i)\vec{s}_j+(\vec{e}_{ij}\cdot\vec{s}_j)\vec{s}_i\big)\right]$$

where $\vec{s}_i$ and $\vec{s}_j$ are the spin on two magnetic particles, r is their separation distance, and the vector $\vec{e}_{ij} = \frac{r_i - r_j}{|r_i - r_j|}$ is the direction vector between the two particles.

Style *spin/dipole/long* computes long-range magnetic dipole-dipole interaction. A *kspace_style* must be defined to use this pair style. Currently, *kspace_style ewald/dipole/spin* and *kspace_style pppm/dipole/spin* support long-range magnetic dipole-dipole interactions.

The *pair_modify* table option is not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

18.408.4 Restrictions

The *spin/dipole/cut* and *spin/dipole/long* styles are part of the SPIN package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Using dipole/spin pair styles with *electron units* is not currently supported.

18.408.5 Related commands

pair_coeff, *kspace_style fix nve/spin*

Default: none

18.409 pair_style spin/dmi command

18.409.1 Syntax

```
pair_style spin/dmi cutoff
```

- cutoff = global cutoff pair (distance in metal units)

18.409.2 Examples

```
pair_style spin/dmi 4.0
pair_coeff * * dmi 2.6 0.001 1.0 0.0 0.0
pair_coeff 1 2 dmi 4.0 0.00109 0.0 0.0 1.0
```

18.409.3 Description

Style *spin/dmi* computes the Dzyaloshinskii-Moriya (DM) interaction between pairs of magnetic spins. According to the expression reported in *(Rohart)*, one has the following DM energy:

$$\mathbf{H}_{dm} = \sum_{i,j=1,i\neq j}^{N} \left(\vec{e}_{ij} \times \vec{D}\right) \cdot \left(\vec{s}_i \times \vec{s}_j\right),$$

where $\vec{s}_i$ and $\vec{s}_j$ are two neighboring magnetic spins of two particles, $\vec{e}_i j = \frac{r_i - r_j}{|r_i - r_j|}$ is the unit vector between sites *i* and *j*, and $\vec{D}$ is the DM vector defining the intensity (in eV) and the direction of the interaction.

In *(Rohart)*, $\vec{D}$ is defined as the direction normal to the film oriented from the high spin-orbit layer to the magnetic ultra-thin film.

The application of a spin-lattice Poisson bracket to this energy (as described in *(Tranchida)*) allows to derive a magnetic torque omega, and a mechanical force F (for spin-lattice calculations only) for each magnetic particle i:

$$\vec{\omega}_i = -\frac{1}{\hbar} \sum_{j}^{Neighb} \vec{s}_j \times \left(\vec{e}_{ij} \times \vec{D}\right) \text{ and } \vec{F}_i = -\sum_{j}^{Neighb} \frac{1}{r_{ij}} \vec{D} \times \left(\vec{s}_i \times \vec{s}_j\right)$$

More details about the derivation of these torques/forces are reported in *(Tranchida)*.

For the *spin/dmi* pair style, the following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, and set in the following order:

- rc (distance units)
- |D| (energy units)
- Dx, Dy, Dz (direction of D)

Note that rc is the radius cutoff of the considered DM interaction, |D| is the norm of the DM vector (in eV), and Dx, Dy and Dz define its direction.

None of those coefficients is optional. If not specified, the *spin/dmi* pair style cannot be used.

18.409.4 Restrictions

All the *pair/spin* styles are part of the SPIN package. These styles are only enabled if LAMMPS was built with this package, and if the atom_style "spin" was declared. See the *Build package* doc page for more info.

18.409.5 Related commands

atom_style spin, *pair_coeff*, *pair_eam*,

Default: none

(Rohart) Rohart and Thiaville, Physical Review B, 88(18), 184422. (2013).

(Tranchida) Tranchida, Plimpton, Thibaudeau and Thompson, Journal of Computational Physics, 372, 406-425, (2018).

18.410 pair_style spin/exchange command

18.410.1 Syntax

```
pair_style spin/exchange cutoff
```

- cutoff = global cutoff pair (distance in metal units)

18.410.2 Examples

```
pair_style spin/exchange 4.0
pair_coeff * * exchange 4.0 0.0446928 0.003496 1.4885
pair_coeff 1 2 exchange 6.0 -0.01575 0.0 1.965
```

18.410.3 Description

Style *spin/exchange* computes the exchange interaction between pairs of magnetic spins:

$$H_{ex} = -\sum_{i,j}^{N} J_{ij}(r_{ij})\, \vec{s}_i \cdot \vec{s}_j$$

where $\vec{s}_i$ and $\vec{s}_j$ are two neighboring magnetic spins of two particles, $r_{ij} = |\vec{r}_i - \vec{r}_j|$ is the inter-atomic distance between the two particles. The summation is over pairs of nearest neighbors. $J(r_{ij})$ is a function defining the intensity and the sign of the exchange interaction for different neighboring shells. This function is defined as:

$$J\left(r_{ij}\right) = 4a\left(\frac{r_{ij}}{d}\right)^2\left(1 - b\left(\frac{r_{ij}}{d}\right)^2\right)e^{-\left(\frac{r_{ij}}{d}\right)^2}\Theta(R_c - r_{ij})$$

where a, b and d are the three constant coefficients defined in the associated "pair_coeff" command, and R_c is the radius cutoff associated to the pair interaction (see below for more explanations).

The coefficients a, b, and d need to be fitted so that the function above matches with the value of the exchange interaction for the N neighbor shells taken into account. Examples and more explanations about this function and its parameterization are reported in *(Tranchida)*.

From this exchange interaction, each spin i will be submitted to a magnetic torque $\vec{\omega}$, and its associated atom can be submitted to a force $\vec{F}$ for spin-lattice calculations (see *fix nve/spin*), such as:

$$\vec{\omega}_i = \frac{1}{\hbar}\sum_{j}^{Neighb} J\left(r_{ij}\right)\, \vec{s}_j \;\text{ and }\; \vec{F}_i = \sum_{j}^{Neighb} \frac{\partial J\left(r_{ij}\right)}{\partial r_{ij}}\left(\vec{s}_i \cdot \vec{s}_j\right)\vec{e}_{ij}$$

with $\hbar$ the Planck constant (in metal units), and $\vec{e}_{ij} = \frac{\vec{r}_i - \vec{r}_j}{|\vec{r}_i - \vec{r}_j|}$ the unit vector between sites i and j.

More details about the derivation of these torques/forces are reported in *(Tranchida)*.

For the *spin/exchange* pair style, the following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, and set in the following order:

- R_c (distance units)
- a (energy units)
- b (adim parameter)

- d (distance units)

Note that R_c is the radius cutoff of the considered exchange interaction, and a, b and d are the three coefficients performing the parameterization of the function $J(r_{ij})$ defined above.

None of those coefficients is optional. If not specified, the *spin/exchange* pair style cannot be used.

18.410.4 Restrictions

All the *pair/spin* styles are part of the SPIN package. These styles are only enabled if LAMMPS was built with this package, and if the atom_style "spin" was declared. See the *Build package* doc page for more info.

18.410.5 Related commands

atom_style spin, *pair_coeff*, *pair_eam*,

Default:

none

(Tranchida) Tranchida, Plimpton, Thibaudeau and Thompson, Journal of Computational Physics, 372, 406-425, (2018).

18.411 pair_style spin/magelec command

18.411.1 Syntax

```
pair_style spin/magelec cutoff
```

- cutoff = global cutoff pair (distance in metal units)

18.411.2 Examples

```
pair_style spin/magelec 4.5
pair_coeff * * magelec 4.5 0.00109 1.0 1.0 1.0
```

18.411.3 Description

Style *spin/me* computes a magneto-electric interaction between pairs of magnetic spins. According to the derivation reported in *(Katsura)*, this interaction is defined as:

$$\vec{\omega}_i = -\frac{1}{\hbar} \sum_j^{Neighb} \vec{s}_j \times \vec{D}(r_{ij})$$

$$\vec{F}_i = -\sum_j^{Neighb} \frac{\partial D(r_{ij})}{\partial r_{ij}} (\vec{s}_i \times \vec{s}_j) \cdot \vec{r}_{ij}$$

where $\vec{s}_i$ and $\vec{s}_j$ are neighboring magnetic spins of two particles.

From this magneto-electric interaction, each spin i will be submitted to a magnetic torque omega, and its associated atom can be submitted to a force F for spin-lattice calculations (see *fix nve/spin*), such as:

$$\vec{F}^i = -\sum_j^{Neighbor} (\vec{s}_i \times \vec{s}_j) \times \vec{E}$$

$$\vec{\omega}^i = -\frac{1}{\hbar} \sum_j^{Neighbor} \vec{s}_j \times \left(\vec{E} \times r_{ij}\right)$$

with h the Planck constant (in metal units) and $\vec{E}$ an electric polarization vector. The norm and direction of E are giving the intensity and the direction of a screened dielectric atomic polarization (in eV).

More details about the derivation of these torques/forces are reported in *(Tranchida)*.

18.411.4 Restrictions

All the *pair/spin* styles are part of the SPIN package. These styles are only enabled if LAMMPS was built with this package, and if the atom_style "spin" was declared. See the *Build package* doc page for more info.

18.411.5 Related commands

atom_style spin, *pair_coeff*, *pair_style spin/exchange*, *pair_eam*,

Default: none

(Katsura) H. Katsura, N. Nagaosa, A.V. Balatsky. Phys. Rev. Lett., 95(5), 057205. (2005)

(Tranchida) Tranchida, Plimpton, Thibaudeau, and Thompson, Journal of Computational Physics, 372, 406-425, (2018).

18.412 pair_style spin/neel command

18.412.1 Syntax

```
pair_style spin/neel cutoff
```

- cutoff = global cutoff pair (distance in metal units)

18.412.2 Examples

```
pair_style spin/neel 4.0
pair_coeff * * neel 4.0 0.0048 0.234 1.168 2.6905 0.705 0.652
pair_coeff 1 2 neel 4.0 0.0048 0.234 1.168 0.0 0.0 1.0
```

18.412.3 Description

Style *spin/neel* computes the Neel pair anisotropy model between pairs of magnetic spins:

$$\mathcal{H}_{N\acute{e}el} = -\sum_{i,j=1,i\neq j}^{N} g_1(r_{ij})\left((\mathbf{e}_{ij}\cdot\mathbf{s}_i)(\mathbf{e}_{ij}\cdot\mathbf{s}_j) - \frac{\mathbf{s}_i\cdot\mathbf{s}_j}{3}\right) + q_1(r_{ij})\left((\mathbf{e}_{ij}\cdot\mathbf{s}_i)^2 - \frac{\mathbf{s}_i\cdot\mathbf{s}_j}{3}\right)\left((\mathbf{e}_{ij}\cdot\mathbf{s}_i)^2 - \frac{\mathbf{s}_i\cdot\mathbf{s}_j}{3}\right) + q_2(r_{ij})\Big((\mathbf{e}_{ij}\cdot\mathbf{s}_i)$$

where $\mathbf{s}_i$ and $\mathbf{s}_j$ are two neighboring magnetic spins of two particles, $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ is the inter-atomic distance between the two particles, $\mathbf{e}_{ij} = \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|}$ is their normalized separation vector and g_1, q_1 and q_2 are three functions defining the intensity of the dipolar and quadrupolar contributions, with:

$$g_1(r_{ij}) = g(r_{ij}) + \frac{12}{35}q(r_{ij})$$
$$q_1(r_{ij}) = \frac{9}{5}q(r_{ij})$$
$$q_2(r_{ij}) = -\frac{2}{5}q(r_{ij})$$

With the functions $g(r_{ij})$ and $q(r_{ij})$ defined and fitted according to the same Bethe-Slater function used to fit the exchange interaction:

$$J\left(r_{ij}\right) = 4a\left(\frac{r_{ij}}{d}\right)^2\left(1 - b\left(\frac{r_{ij}}{d}\right)^2\right)e^{-\left(\frac{r_{ij}}{d}\right)^2}\Theta(R_c - r_{ij})$$

where a, b and d are the three constant coefficients defined in the associated "pair_coeff" command.

The coefficients a, b, and d need to be fitted so that the function above matches with the values of the magneto-elastic constant of the materials at stake.

Examples and more explanations about this function and its parameterization are reported in *(Tranchida)*. More examples of parameterization will be provided in future work.

From this DM interaction, each spin i will be submitted to a magnetic torque ω and its associated atom to a force $\mathbf{F}$ (for spin-lattice calculations only).

More details about the derivation of these torques/forces are reported in *(Tranchida)*.

18.412.4 Restrictions

All the *pair/spin* styles are part of the SPIN package. These styles are only enabled if LAMMPS was built with this package, and if the atom_style "spin" was declared. See the *Build package* doc page for more info.

18.412.5 Related commands

atom_style spin, *pair_coeff*, *pair_eam*,

Default:

none

(Tranchida) Tranchida, Plimpton, Thibaudeau and Thompson, Journal of Computational Physics, 372, 406-425, (2018).

18.413 pair_style srp command

18.413.1 Syntax

```
pair_style srp cutoff btype dist keyword value ...
```

- cutoff = global cutoff for SRP interactions (distance units)
- btype = bond type to apply SRP interactions to (can be wildcard, see below)
- distance = *min* or *mid*
- zero or more keyword/value pairs may be appended
- keyword = *exclude*

  bptype value = atom type for bond particles
  exclude value = *yes* or *no*

18.413.2 Examples

```
pair_style hybrid dpd 1.0 1.0 12345 srp 0.8 1 mid exclude yes
pair_coeff 1 1 dpd 60.0 4.5 1.0
pair_coeff 1 2 none
pair_coeff 2 2 srp 100.0 0.8

pair_style hybrid dpd 1.0 1.0 12345 srp 0.8 \* min exclude yes
pair_coeff 1 1 dpd 60.0 50 1.0
pair_coeff 1 2 none
pair_coeff 2 2 srp 40.0

pair_style hybrid srp 0.8 2 mid
pair_coeff 1 1 none
pair_coeff 1 2 none
pair_coeff 2 2 srp 100.0 0.8
```

18.413.3 Description

Style *srp* computes a soft segmental repulsive potential (SRP) that acts between pairs of bonds. This potential is useful for preventing bonds from passing through one another when a soft non-bonded potential acts between beads in, for example, DPD polymer chains. An example input script that uses this command is provided in examples/USER/srp.

Bonds of specified type *btype* interact with one another through a bond-pairwise potential, such that the force on bond *i* due to bond *j* is as follows

$$F_{ij}^{SRP} = C(1 - r/r_c)\hat{r}_{ij} \qquad r < r_c$$

where *r* and $\hat{r}_{ij}$ are the distance and unit vector between the two bonds. Note that *btype* can be specified as an asterisk "*", which case the interaction is applied to all bond types. The *mid* option computes *r* and $\hat{r}_{ij}$ from the midpoint distance between bonds. The *min* option computes *r* and $\hat{r}_{ij}$ from the minimum distance between bonds. The force acting on a bond is mapped onto the two bond atoms according to the lever rule,

$$F_{i1}^{SRP} = F_{ij}^{SRP}(L)$$
$$F_{i2}^{SRP} = F_{ij}^{SRP}(1 - L)$$

where L is the normalized distance from the atom to the point of closest approach of bond i and j. The *mid* option takes L as 0.5 for each interaction as described in *(Sirk)*.

The following coefficients must be defined via the *pair_coeff* command as in the examples above, or in the data file or restart file read by the *read_data* or *read_restart* commands:

- C (force units)
- r_c (distance units)

The last coefficient is optional. If not specified, the global cutoff is used.

Note: Pair style srp considers each bond of type *btype* to be a fictitious "particle" of type *bptype*, where *bptype* is either the largest atom type in the system, or the type set by the *bptype* flag. Any actual existing particles with this atom type will be deleted at the beginning of a run. This means you must specify the number of types in your system accordingly; usually to be one larger than what would normally be the case, e.g. via the *create_box* or by changing the header in your *data file*. The fictitious "bond particles" are inserted at the beginning of the run, and serve as placeholders that define the position of the bonds. This allows neighbor lists to be constructed and pairwise interactions to be computed in almost the same way as is done for actual particles. Because bonds interact only with other bonds, *pair_style hybrid* should be used to turn off interactions between atom type *bptype* and all other types of atoms. An error will be flagged if *pair_style hybrid* is not used.

The optional *exclude* keyword determines if forces are computed between first neighbor (directly connected) bonds. For a setting of *no*, first neighbor forces are computed; for *yes* they are not computed. A setting of *no* cannot be used with the *min* option for distance calculation because the minimum distance between directly connected bonds is zero.

Pair style *srp* turns off normalization of thermodynamic properties by particle number, as if the command *thermo_modify norm no* had been issued.

The pairwise energy associated with style *srp* is shifted to be zero at the cutoff distance r_c.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair styles does not support mixing.

This pair style does not support the *pair_modify* shift option for the energy of the pair interaction. Note that as discussed above, the energy term is already shifted to be 0.0 at the cutoff distance r_c.

The *pair_modify* table option is not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

This pair style writes global and per-atom information to *binary restart files*. Pair srp should be used with *pair_style hybrid*, thus the pair_coeff commands need to be specified in the input script when reading a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.413.4 Restrictions

This pair style is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This pair style must be used with *pair_style hybrid*.

This pair style requires the *newton* command to be *on* for non-bonded interactions.

This pair style is not compatible with *rigid body integrators*

18.413.5 Related commands

pair_style hybrid, *pair_coeff*, *pair dpd*

18.413.6 Default

The default keyword value is exclude = yes.

(Sirk) Sirk TW, Sliozberg YR, Brennan JK, Lisal M, Andzelm JW, J Chem Phys, 136 (13) 134903, 2012.

18.414 pair_style sw command

18.415 pair_style sw/gpu command

18.416 pair_style sw/intel command

18.417 pair_style sw/kk command

18.418 pair_style sw/omp command

18.418.1 Syntax

```
pair_style sw
```

18.418.2 Examples

```
pair_style sw
pair_coeff * * si.sw Si
pair_coeff * * GaN.sw Ga N Ga
```

18.418.3 Description

The *sw* style computes a 3-body *Stillinger-Weber* potential for the energy E of a system of atoms as

$$E = \sum_i \sum_{j>i} \phi_2(r_{ij}) + \sum_i \sum_{j \neq i} \sum_{k>j} \phi_3(r_{ij}, r_{ik}, \theta_{ijk})$$

$$\phi_2(r_{ij}) = A_{ij}\epsilon_{ij} \left[B_{ij}(\frac{\sigma_{ij}}{r_{ij}})^{p_{ij}} - (\frac{\sigma_{ij}}{r_{ij}})^{q_{ij}} \right] \exp\left(\frac{\sigma_{ij}}{r_{ij} - a_{ij}\sigma_{ij}} \right)$$

$$\phi_3(r_{ij}, r_{ik}, \theta_{ijk}) = \lambda_{ijk}\epsilon_{ijk} \left[\cos\theta_{ijk} - \cos\theta_{0ijk}\right]^2 \exp\left(\frac{\gamma_{ij}\sigma_{ij}}{r_{ij} - a_{ij}\sigma_{ij}} \right) \exp\left(\frac{\gamma_{ik}\sigma_{ik}}{r_{ik} - a_{ik}\sigma_{ik}} \right)$$

where ϕ_2 is a two-body term and ϕ_3 is a three-body term. The summations in the formula are over all neighbors J and K of atom I within a cutoff distance a.

Only a single pair_coeff command is used with the *sw* style which specifies a Stillinger-Weber potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of SW elements to atom types

See the *pair_coeff* doc page for alternate ways to specify the path for the potential file.

As an example, imagine a file SiC.sw has Stillinger-Weber values for Si and C. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * SiC.sw Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the SW file. The final C argument maps LAMMPS atom type 4 to the C element in the SW file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *sw* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Stillinger-Weber files in the *potentials* directory of the LAMMPS distribution have a ".sw" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements. The parameters in a single entry correspond to the two-body and three-body coefficients in the formula above:

- element 1 (the center atom in a 3-body interaction)
- element 2
- element 3
- ϵ (energy units)
- σ (distance units)
- a
- λ
- γ
- $\cos\theta_0$
- A
- B
- p
- q

- tol

The A, B, p, and q parameters are used only for two-body interactions. The λ and $\cos\theta_0$ parameters are used only for three-body interactions. The ϵ, σ and a parameters are used for both two-body and three-body interactions. γ is used only in the three-body interactions, but is defined for pairs of atoms. The non-annotated parameters are unitless.

LAMMPS introduces an additional performance-optimization parameter tol that is used for both two-body and three-body interactions. In the Stillinger-Weber potential, the interaction energies become negligibly small at atomic separations substantially less than the theoretical cutoff distances. LAMMPS therefore defines a virtual cutoff distance based on a user defined tolerance tol. The use of the virtual cutoff distance in constructing atom neighbor lists can significantly reduce the neighbor list sizes and therefore the computational cost. LAMMPS provides a *tol* value for each of the three-body entries so that they can be separately controlled. If tol = 0.0, then the standard Stillinger-Weber cutoff is used.

The Stillinger-Weber potential file must contain entries for all the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries.

For a single-element simulation, only a single entry is required (e.g. SiSiSi). For a two-element simulation, the file must contain 8 entries (for SiSiSi, SiSiC, SiCSi, SiCC, CSiSi, CSiC, CCSi, CCC), that specify SW parameters for all permutations of the two elements interacting in three-body configurations. Thus for 3 elements, 27 entries would be required, etc.

As annotated above, the first element in the entry is the center atom in a three-body interaction. Thus an entry for SiCC means a Si atom with 2 C atoms as neighbors. The parameter values used for the two-body interaction come from the entry where the 2nd and 3rd elements are the same. Thus the two-body parameters for Si interacting with C, comes from the SiCC entry. The three-body parameters can in principle be specific to the three elements of the configuration. In the literature, however, the three-body parameters are usually defined by simple formulas involving two sets of pair-wise parameters, corresponding to the ij and ik pairs, where i is the center atom. The user must ensure that the correct combining rule is used to calculate the values of the three-body parameters for alloys. Note also that the function ϕ_3 contains two exponential screening factors with parameter values from the ij pair and ik pairs. So ϕ_3 for a C atom bonded to a Si atom and a second C atom will depend on the three-body parameters for the CSiC entry, and also on the two-body parameters for the CCC and CSiSi entries. Since the order of the two neighbors is arbitrary, the three-body parameters for entries CSiC and CCSi should be the same. Similarly, the two-body parameters for entries SiCC and CSiSi should also be the same. The parameters used only for two-body interactions (A, B, p, and q) in entries whose 2nd and 3rd element are different (e.g. SiCSi) are not used for anything and can be set to 0.0 if desired. This is also true for the parameters in ϕ_3 that are taken from the ij and ik pairs (σ, a, γ)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

When using the USER-INTEL package with this style, there is an additional 5 to 10 percent performance improvement when the Stillinger-Weber parameters p and q are set to 4 and 0 respectively. These parameters are common for modeling silicon and water.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above from values in the potential file.

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.418.4 Restrictions

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This pair style requires the *newton* setting to be "on" for pair interactions.

The Stillinger-Weber potential files provided with LAMMPS (see the potentials directory) are parameterized for metal *units*. You can use the SW potential with any LAMMPS units, but you would need to create your own SW potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

18.418.5 Related commands

pair_coeff

Default: none

(Stillinger) Stillinger and Weber, Phys Rev B, 31, 5262 (1985).

18.419 pair_style table command

18.420 pair_style table/gpu command

18.421 pair_style table/kk command

18.422 pair_style table/omp command

18.422.1 Syntax

```
pair_style table style N keyword ...
```

- style = *lookup* or *linear* or *spline* or *bitmap* = method of interpolation
- N = use N values in *lookup*, *linear*, *spline* tables
- N = use 2^N values in *bitmap* tables
- zero or more keywords may be appended
- keyword = *ewald* or *pppm* or *msm* or *dispersion* or *tip4p*

18.422.2 Examples

```
pair_style table linear 1000
pair_style table linear 1000 pppm
pair_style table bitmap 12
pair_coeff * 3 morse.table ENTRY1
pair_coeff * 3 morse.table ENTRY1 7.0
```

18.422.3 Description

Style *table* creates interpolation tables from potential energy and force values listed in a file(s) as a function of distance. When performing dynamics or minimization, the interpolation tables are used to evaluate energy and forces for pairwise interactions between particles, similar to how analytic formulas are used for other pair styles.

The interpolation tables are created as a pre-computation by fitting cubic splines to the file values and interpolating energy and force values at each of N distances. During a simulation, the tables are used to interpolate energy and force values as needed for each pair of particles separated by a distance R. The interpolation is done in one of 4 styles: *lookup*, *linear*, *spline*, or *bitmap*.

For the *lookup* style, the distance R is used to find the nearest table entry, which is the energy or force.

For the *linear* style, the distance R is used to find the 2 surrounding table values from which an energy or force is computed by linear interpolation.

For the *spline* style, a cubic spline coefficients are computed and stored for each of the N values in the table, one set of splines for energy, another for force. Note that these splines are different than the ones used to pre-compute the N values. Those splines were fit to the *Nfile* values in the tabulated file, where often $Nfile < N$. The distance R is used to find the appropriate set of spline coefficients which are used to evaluate a cubic polynomial which computes the energy or force.

For the *bitmap* style, the specified N is used to create interpolation tables that are 2^N in length. The distance R is used to index into the table via a fast bit-mapping technique due to *(Wolff)*, and a linear interpolation is performed between adjacent table values.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above.

- filename
- keyword
- cutoff (distance units)

The filename specifies a file containing tabulated energy and force values. The keyword specifies a section of the file. The cutoff is an optional coefficient. If not specified, the outer cutoff in the table itself (see below) will be used to build an interpolation table that extend to the largest tabulated distance. If specified, only file values up to the cutoff are used to create the interpolation table. The format of this file is described below.

If your tabulated potential(s) are designed to be used as the short-range part of one of the long-range solvers specified by the *kspace_style* command, then you must use one or more of the optional keywords listed above for the pair_style command. These are *ewald* or *pppm* or *msm* or *dispersion* or *tip4p*. This is so LAMMPS can insure the short-range potential and long-range solver are compatible with each other, as it does for other short-range pair styles, such as *pair_style lj/cut/coul/long*. Note that it is up to you to insure the tabulated values for each pair of atom types has the correct functional form to be compatible with the matching long-range solver.

Here are some guidelines for using the pair_style table command to best effect:

- Vary the number of table points; you may need to use more than you think to get good resolution.

- Always use the *pair_write* command to produce a plot of what the final interpolated potential looks like. This can show up interpolation "features" you may not like.
- Start with the linear style; it's the style least likely to have problems.
- Use *N* in the pair_style command equal to the "N" in the tabulation file, and use the "RSQ" or "BITMAP" parameter, so additional interpolation is not needed. See discussion below.
- Make sure that your tabulated forces and tabulated energies are consistent (dE/dr = -F) over the entire range of r values. LAMMPS will warn if this is not the case.
- Use as large an inner cutoff as possible. This avoids fitting splines to very steep parts of the potential.

The format of a tabulated file is a series of one or more sections, defined as follows (without the parenthesized comments):

```
# Morse potential for Fe   (one or more comment or blank lines)

MORSE_FE                   (keyword is first text on line)
N 500 R 1.0 10.0           (N, R, RSQ, BITMAP, FPRIME parameters)
                           (blank)
1 1.0 25.5 102.34          (index, r, energy, force)
2 1.02 23.4 98.5
...
500 10.0 0.001 0.003
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the pair_coeff command. The next line lists (in any order) one or more parameters for the table. Each parameter is a keyword followed by one or more numeric values.

The parameter "N" is required and its value is the number of table entries that follow. Note that this may be different than the *N* specified in the *pair_style table* command. Let Ntable = *N* in the pair_style command, and Nfile = "N" in the tabulated file. What LAMMPS does is a preliminary interpolation by creating splines using the Nfile tabulated values as nodal points. It uses these to interpolate energy and force values at Ntable different points. The resulting tables of length Ntable are then used as described above, when computing energy and force for individual pair distances. This means that if you want the interpolation tables of length Ntable to match exactly what is in the tabulated file (with effectively no preliminary interpolation), you should set Ntable = Nfile, and use the "RSQ" or "BITMAP" parameter. This is because the internal table abscissa is always RSQ (separation distance squared), for efficient lookup.

All other parameters are optional. If "R" or "RSQ" or "BITMAP" does not appear, then the distances in each line of the table are used as-is to perform spline interpolation. In this case, the table values can be spaced in *r* uniformly or however you wish to position table values in regions of large gradients.

If used, the parameters "R" or "RSQ" are followed by 2 values *rlo* and *rhi*. If specified, the distance associated with each energy and force value is computed from these 2 values (at high accuracy), rather than using the (low-accuracy) value listed in each line of the table. The distance values in the table file are ignored in this case. For "R", distances uniformly spaced between *rlo* and *rhi* are computed; for "RSQ", squared distances uniformly spaced between *rlo*rlo* and *rhi*rhi* are computed.

Note: If you use "R" or "RSQ", the tabulated distance values in the file are effectively ignored, and replaced by new values as described in the previous paragraph. If the distance value in the table is not very close to the new value (i.e. round-off difference), then you will be assigning energy/force values to a different distance, which is probably not what you want. LAMMPS will warn if this is occurring.

If used, the parameter "BITMAP" is also followed by 2 values *rlo* and *rhi*. These values, along with the "N" value determine the ordering of the N lines that follow and what distance is associated with each. This ordering is complex, so it is not documented here, since this file is typically produced by the *pair_write* command with its *bitmap* option. When the table is in BITMAP format, the "N" parameter in the file must be equal to 2^M where M is the value specified in the pair_style command. Also, a cutoff parameter cannot be used as an optional 3rd argument in the pair_coeff command; the entire table extent as specified in the file must be used.

If used, the parameter "FPRIME" is followed by 2 values *fplo* and *fphi* which are the derivative of the force at the innermost and outermost distances listed in the table. These values are needed by the spline construction routines. If not specified by the "FPRIME" parameter, they are estimated (less accurately) by the first 2 and last 2 force values in the table. This parameter is not used by BITMAP tables.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is r (in distance units), the 3rd value is the energy (in energy units), and the 4th is the force (in force units). The r values must increase from one line to the next (unless the BITMAP parameter is specified).

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

The *pair_modify* shift, table, and tail options are not relevant for this pair style.

This pair style writes the settings for the "pair_style table" command to *binary restart files*, so a pair_style command does not need to specified in an input script that reads a restart file. However, the coefficient information is not stored in the restart file, since it is tabulated in the potential files. Thus, pair_coeff commands do need to be specified in the restart input script.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.422.4 Restrictions

none

18.422.5 Related commands

pair_coeff, *pair_write*

Default: none

(Wolff) Wolff and Rudd, Comp Phys Comm, 120, 200-32 (1999).

18.423 pair_style table/rx command

18.424 pair_style table/rx/kk command

18.424.1 Syntax

```
pair_style table style N ...
```

- style = *lookup* or *linear* or *spline* or *bitmap* = method of interpolation
- N = use N values in *lookup*, *linear*, *spline* tables
- weighting = fractional or molecular (optional)

18.424.2 Examples

```
pair_style table/rx linear 1000
pair_style table/rx linear 1000 fractional
pair_style table/rx linear 1000 molecular
pair_coeff * * rxn.table ENTRY1 h2o h2o 10.0
pair_coeff * * rxn.table ENTRY1 1fluid 1fluid 10.0
pair_coeff * 3 rxn.table ENTRY1 h2o no2 10.0
```

18.424.3 Description

Style *table/rx* is used in reaction DPD simulations,where the coarse-grained (CG) particles are composed of *m* species whose reaction rate kinetics are determined from a set of *n* reaction rate equations through the *fix rx* command. The species of one CG particle can interact with a species in a neighboring CG particle through a site-site interaction potential model. Style *table/rx* creates interpolation tables of length *N* from pair potential and force values listed in a file(s) as a function of distance. The files are read by the *pair_coeff* command.

The interpolation tables are created by fitting cubic splines to the file values and interpolating energy and force values at each of *N* distances. During a simulation, these tables are used to interpolate energy and force values as needed. The interpolation is done in one of 4 styles: *lookup*, *linear*, *spline*, or *bitmap*.

For the *lookup* style, the distance between 2 atoms is used to find the nearest table entry, which is the energy or force.

For the *linear* style, the pair distance is used to find 2 surrounding table values from which an energy or force is computed by linear interpolation.

For the *spline* style, a cubic spline coefficients are computed and stored at each of the *N* values in the table. The pair distance is used to find the appropriate set of coefficients which are used to evaluate a cubic polynomial which computes the energy or force.

For the *bitmap* style, the N means to create interpolation tables that are 2^N in length. The pair distance is used to index into the table via a fast bit-mapping technique *(Wolff)* and a linear interpolation is performed between adjacent table values.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above.

- filename
- keyword
- species1
- species2
- cutoff (distance units)

The filename specifies a file containing tabulated energy and force values. The keyword specifies a section of the file. The cutoff is an optional coefficient. If not specified, the outer cutoff in the table itself (see below) will be used to build an interpolation table that extend to the largest tabulated distance. If specified, only file values up to the cutoff are used to create the interpolation table. The format of this file is described below.

The species tags define the site-site interaction potential between two species contained within two different particles. The species tags must either correspond to the species defined in the reaction kinetics files specified with the *fix rx* command or they must correspond to the tag "1fluid", signifying interaction with a product species mixture determined through a one-fluid approximation. The interaction potential is weighted by the geometric average of either the mole fraction concentrations or the number of molecules associated with the interacting coarse-grained particles (see the *fractional* or *molecular* weighting pair style options). The coarse-grained potential is stored before and after the reaction kinetics solver is applied, where the difference is defined to be the internal chemical energy (uChem).

Here are some guidelines for using the pair_style table/rx command to best effect:

- Vary the number of table points; you may need to use more than you think to get good resolution.
- Always use the *pair_write* command to produce a plot of what the final interpolated potential looks like. This can show up interpolation "features" you may not like.
- Start with the linear style; it's the style least likely to have problems.
- Use *N* in the pair_style command equal to the "N" in the tabulation file, and use the "RSQ" or "BITMAP" parameter, so additional interpolation is not needed. See discussion below.
- Make sure that your tabulated forces and tabulated energies are consistent (dE/dr = -F) along the entire range of r values.
- Use as large an inner cutoff as possible. This avoids fitting splines to very steep parts of the potential.

The format of a tabulated file is a series of one or more sections, defined as follows (without the parenthesized comments):

```
# Morse potential for Fe   (one or more comment or blank lines)

MORSE_FE                   (keyword is first text on line)
N 500 R 1.0 10.0           (N, R, RSQ, BITMAP, FPRIME parameters)
                           (blank)
1 1.0 25.5 102.34          (index, r, energy, force)
2 1.02 23.4 98.5
...
500 10.0 0.001 0.003
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the pair_coeff command. The next line lists (in any order) one or more parameters for the table. Each parameter is a keyword followed by one or more numeric values.

The parameter "N" is required and its value is the number of table entries that follow. Note that this may be different than the *N* specified in the *pair_style table/rx* command. Let Ntable = *N* in the pair_style command, and Nfile = "N" in the tabulated file. What LAMMPS does is a preliminary interpolation by creating splines using the Nfile tabulated values as nodal points. It uses these to interpolate as needed to generate energy and force values at Ntable different points. The resulting tables of length Ntable are then used as described above, when computing energy and force for individual pair distances. This means that if you want the interpolation tables of length Ntable to match exactly what is in the tabulated file (with effectively no preliminary interpolation), you should set Ntable = Nfile, and use the "RSQ" or "BITMAP" parameter. The internal table abscissa is RSQ (separation distance squared).

All other parameters are optional. If "R" or "RSQ" or "BITMAP" does not appear, then the distances in each line of the table are used as-is to perform spline interpolation. In this case, the table values can be spaced in *r* uniformly or however you wish to position table values in regions of large gradients.

If used, the parameters "R" or "RSQ" are followed by 2 values *rlo* and *rhi*. If specified, the distance associated with each energy and force value is computed from these 2 values (at high accuracy), rather than using the (low-accuracy) value listed in each line of the table. The distance values in the table file are ignored in this case. For "R", distances uniformly spaced between *rlo* and *rhi* are computed; for "RSQ", squared distances uniformly spaced between *rlo*rlo* and *rhi*rhi* are computed.

If used, the parameter "BITMAP" is also followed by 2 values *rlo* and *rhi*. These values, along with the "N" value determine the ordering of the N lines that follow and what distance is associated with each. This ordering is complex, so it is not documented here, since this file is typically produced by the *pair_write* command with its *bitmap* option. When the table is in BITMAP format, the "N" parameter in the file must be equal to 2^M where M is the value specified in the pair_style command. Also, a cutoff parameter cannot be used as an optional 3rd argument in the pair_coeff command; the entire table extent as specified in the file must be used.

If used, the parameter "FPRIME" is followed by 2 values *fplo* and *fphi* which are the derivative of the force at the innermost and outermost distances listed in the table. These values are needed by the spline construction routines. If not specified by the "FPRIME" parameter, they are estimated (less accurately) by the first 2 and last 2 force values in the table. This parameter is not used by BITMAP tables.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is r (in distance units), the 3rd value is the energy (in energy units), and the 4th is the force (in force units). The r values must increase from one line to the next (unless the BITMAP parameter is specified).

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

The *pair_modify* shift, table, and tail options are not relevant for this pair style.

This pair style writes the settings for the "pair_style table/rx" command to *binary restart files*, so a pair_style command does not need to specified in an input script that reads a restart file. However, the coefficient information is not stored in the restart file, since it is tabulated in the potential files. Thus, pair_coeff commands do need to be specified in the restart input script.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

18.424.4 Restrictions

This command is part of the USER-DPD package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

18.424.5 Related commands

pair_coeff

Default: fractional weighting

(Wolff) Wolff and Rudd, Comp Phys Comm, 120, 200-32 (1999).

18.425 pair_style tersoff command

18.426 pair_style tersoff/table command

18.427 pair_style tersoff/gpu command

18.428 pair_style tersoff/intel command

18.429 pair_style tersoff/kk command

18.430 pair_style tersoff/omp command

18.431 pair_style tersoff/table/omp command

18.431.1 Syntax

```
pair_style style
```

- style = *tersoff* or *tersoff/table* or *tersoff/gpu* or *tersoff/omp* or *tersoff/table/omp*

18.431.2 Examples

```
pair_style tersoff
pair_coeff * * Si.tersoff Si
pair_coeff * * SiC.tersoff Si C Si

pair_style tersoff/table
pair_coeff * * SiCGe.tersoff Si(D)
```

18.431.3 Description

The *tersoff* style computes a 3-body Tersoff potential *(Tersoff_1)* for the energy E of a system of atoms as

$$
\begin{aligned}
E &= \frac{1}{2}\sum_i \sum_{j\neq i} V_{ij} \\
V_{ij} &= f_C(r_{ij})\left[f_R(r_{ij}) + b_{ij} f_A(r_{ij})\right] \\
f_C(r) &= \begin{cases} 1 & : \quad r < R - D \\ \frac{1}{2} - \frac{1}{2}\sin\left(\frac{\pi}{2}\frac{r-R}{D}\right) & : \quad R - D < r < R + D \\ 0 & : \quad r > R + D \end{cases} \\
f_R(r) &= A\exp(-\lambda_1 r) \\
f_A(r) &= -B\exp(-\lambda_2 r) \\
b_{ij} &= (1 + \beta^n {\zeta_{ij}}^n)^{-\frac{1}{2n}} \\
\zeta_{ij} &= \sum_{k\neq i,j} f_C(r_{ik}) g(\theta_{ijk}) \exp\left[{\lambda_3}^m (r_{ij} - r_{ik})^m\right] \\
g(\theta) &= \gamma_{ijk}\left(1 + \frac{c^2}{d^2} - \frac{c^2}{[d^2 + (\cos\theta - \cos\theta_0)^2]}\right)
\end{aligned}
$$

where f_R is a two-body term and f_A includes three-body interactions. The summations in the formula are over all neighbors J and K of atom I within a cutoff distance = R + D.

The *tersoff/table* style uses tabulated forms for the two-body, environment and angular functions. Linear interpolation is performed between adjacent table entries. The table length is chosen to be accurate within 10^-6 with respect to the *tersoff* style energy. The *tersoff/table* should give better performance in terms of speed.

Only a single pair_coeff command is used with the *tersoff* style which specifies a Tersoff potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of Tersoff elements to atom types

See the *pair_coeff* doc page for alternate ways to specify the path for the potential file.

As an example, imagine the SiC.tersoff file has Tersoff values for Si and C. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * SiC.tersoff Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the Tersoff file. The final C argument maps LAMMPS atom type 4 to the C element in the Tersoff file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *tersoff* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Tersoff files in the *potentials* directory of the LAMMPS distribution have a ".tersoff" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements. The parameters in a single entry correspond to coefficients in the formula above:

- element 1 (the center atom in a 3-body interaction)
- element 2 (the atom bonded to the center atom)
- element 3 (the atom influencing the 1-2 bond in a bond-order sense)
- m

- γ
- λ_3 (1/distance units)
- c
- d
- $\cos\theta_0$ (can be a value < -1 or > 1)
- n
- β
- λ_2 (1/distance units)
- B (energy units)
- R (distance units)
- D (distance units)
- λ_1 (1/distance units)
- A (energy units)

The n, β, λ_2, B, λ_1, and A parameters are only used for two-body interactions. The m, γ, λ_3, c, d, and $\cos\theta_0$ parameters are only used for three-body interactions. The R and D parameters are used for both two-body and three-body interactions. The non-annotated parameters are unitless. The value of m must be 3 or 1.

The Tersoff potential file must contain entries for all the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries.

For a single-element simulation, only a single entry is required (e.g. SiSiSi). For a two-element simulation, the file must contain 8 entries (for SiSiSi, SiSiC, SiCSi, SiCC, CSiSi, CSiC, CCSi, CCC), that specify Tersoff parameters for all permutations of the two elements interacting in three-body configurations. Thus for 3 elements, 27 entries would be required, etc.

As annotated above, the first element in the entry is the center atom in a three-body interaction and it is bonded to the 2nd atom and the bond is influenced by the 3rd atom. Thus an entry for SiCC means Si bonded to a C with another C atom influencing the bond. Thus three-body parameters for SiCSi and SiSiC entries will not, in general, be the same. The parameters used for the two-body interaction come from the entry where the 2nd element is repeated. Thus the two-body parameters for Si interacting with C, comes from the SiCC entry.

The parameters used for a particular three-body interaction come from the entry with the corresponding three elements. The parameters used only for two-body interactions (n, β, λ_2, B, λ_1, and A) in entries whose 2nd and 3rd element are different (e.g. SiCSi) are not used for anything and can be set to 0.0 if desired.

Note that the twobody parameters in entries such as SiCC and CSiSi are often the same, due to the common use of symmetric mixing rules, but this is not always the case. For example, the beta and n parameters in Tersoff_2 *(Tersoff_2)* are not symmetric.

We chose the above form so as to enable users to define all commonly used variants of the Tersoff potential. In particular, our form reduces to the original Tersoff form when m = 3 and gamma = 1, while it reduces to the form of *Albe et al.* when beta = 1 and m = 1. Note that in the current Tersoff implementation in LAMMPS, m must be specified as either 3 or 1. Tersoff used a slightly different but equivalent form for alloys, which we will refer to as Tersoff_2 potential *(Tersoff_2)*. The *tersoff/table* style implements Tersoff_2 parameterization only.

LAMMPS parameter values for Tersoff_2 can be obtained as follows: $\gamma_{ijk} = \omega_{ik}$, $\lambda_3 = 0$ and the value of m has no

effect. The parameters for species i and j can be calculated using the Tersoff_2 mixing rules:

$$\lambda_1^{i,j} = \frac{1}{2}(\lambda_1^i + \lambda_1^j)$$
$$\lambda_2^{i,j} = \frac{1}{2}(\lambda_2^i + \lambda_2^j)$$
$$A_{i,j} = (A_i A_j)^{1/2}$$
$$B_{i,j} = \chi_{ij}(B_i B_j)^{1/2}$$
$$R_{i,j} = (R_i R_j)^{1/2}$$
$$S_{i,j} = (S_i S_j)^{1/2}$$

Tersoff_2 parameters R and S must be converted to the LAMMPS parameters R and D (R is different in both forms), using the following relations: R=(R'+S')/2 and D=(S'-R')/2, where the primes indicate the Tersoff_2 parameters.

In the potentials directory, the file SiCGe.tersoff provides the LAMMPS parameters for Tersoff's various versions of Si, as well as his alloy parameters for Si, C, and Ge. This file can be used for pure Si, (three different versions), pure C, pure Ge, binary SiC, and binary SiGe. LAMMPS will generate an error if this file is used with any combination involving C and Ge, since there are no entries for the GeC interactions (Tersoff did not publish parameters for this cross-interaction.) Tersoff files are also provided for the SiC alloy (SiC.tersoff) and the GaN (GaN.tersoff) alloys.

Many thanks to Rutuparna Narulkar, David Farrell, and Xiaowang Zhou for helping clarify how Tersoff parameters for alloys have been defined in various papers.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above from values in the potential file.

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.431.4 Restrictions

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This pair style requires the *newton* setting to be "on" for pair interactions.

The Tersoff potential files provided with LAMMPS (see the potentials directory) are parameterized for metal *units*. You can use the Tersoff potential with any LAMMPS units, but you would need to create your own Tersoff potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

18.431.5 Related commands

pair_coeff

Default: none

(Tersoff_1) J. Tersoff, Phys Rev B, 37, 6991 (1988).

(Albe) J. Nord, K. Albe, P. Erhart, and K. Nordlund, J. Phys.: Condens. Matter, 15, 5649(2003).

(Tersoff_2) J. Tersoff, Phys Rev B, 39, 5566 (1989); errata (PRB 41, 3248)

18.432 pair_style tersoff/mod command

18.433 pair_style tersoff/mod/c command

18.434 pair_style tersoff/mod/gpu command

18.435 pair_style tersoff/mod/kk command

18.436 pair_style tersoff/mod/omp command

18.437 pair_style tersoff/mod/c/omp command

18.437.1 Syntax

```
pair_style tersoff/mod

pair_style tersoff/mod/c
```

18.437.2 Examples

```
pair_style tersoff/mod
pair_coeff * * Si.tersoff.mod Si Si

pair_style tersoff/mod/c
pair_coeff * * Si.tersoff.modc Si Si
```

18.437.3 Description

The *tersoff/mod* and *tersoff/mod/c* styles computes a bond-order type interatomic potential *(Kumagai)* based on a 3-body Tersoff potential *(Tersoff_1)*, *(Tersoff_2)* with modified cutoff function and angular-dependent term, giving the energy E of a system of atoms as

$$
\begin{aligned}
E &= \frac{1}{2}\sum_i \sum_{j\neq i} V_{ij} \\
V_{ij} &= f_C(r_{ij})\left[f_R(r_{ij}) + b_{ij} f_A(r_{ij})\right] \\
f_C(r) &= \begin{cases} 1 & : \quad r < R - D \\ \frac{1}{2} - \frac{9}{16}\sin\left(\frac{\pi}{2}\frac{r-R}{D}\right) - \frac{1}{16}\sin\left(\frac{3\pi}{2}\frac{r-R}{D}\right) & : \quad R - D < r < R + D \\ 0 & : \quad r > R + D \end{cases} \\
f_R(r) &= A\exp(-\lambda_1 r) \\
f_A(r) &= -B\exp(-\lambda_2 r) \\
b_{ij} &= (1 + {\zeta_{ij}}^{\eta})^{-\frac{1}{2n}} \\
\zeta_{ij} &= \sum_{k\neq i,j} f_C(r_{ik}) g(\theta_{ijk}) \exp\left[\alpha(r_{ij} - r_{ik})^{\beta}\right] \\
g(\theta) &= c_1 + g_o(\theta) g_a(\theta) \\
g_o(\theta) &= \frac{c_2(h - \cos\theta)^2}{c_3 + (h - \cos\theta)^2} \\
g_a(\theta) &= 1 + c_4 \exp\left[-c_5(h - \cos\theta)^2\right]
\end{aligned}
$$

where f_R is a two-body term and f_A includes three-body interactions. The summations in the formula are over all neighbors J and K of atom I within a cutoff distance = R + D. The *tersoff/mod/c* style differs from *tersoff/mod* only in the formulation of the V_ij term, where it contains an additional c0 term.

$$V_{ij} = f_C(r_{ij})\left[f_R(r_{ij}) + b_{ij} f_A(r_{ij}) + c_0\right]$$

The modified cutoff function f_C proposed by *(Murty)* and having a continuous second-order differential is employed. The angular-dependent term $g(\theta)$ was modified to increase the flexibility of the potential.

The *tersoff/mod* potential is fitted to both the elastic constants and melting point by employing the modified Tersoff potential function form in which the angular-dependent term is improved. The model performs extremely well in describing the crystalline, liquid, and amorphous phases *(Schelling)*.

Only a single pair_coeff command is used with the *tersoff/mod* style which specifies a Tersoff/MOD potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of Tersoff/MOD elements to atom types

As an example, imagine the Si.tersoff_mod file has Tersoff values for Si. If your LAMMPS simulation has 3 Si atoms types, you would use the following pair_coeff command:

```
pair_coeff * * Si.tersoff_mod Si Si Si
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the Tersoff/MOD file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *tersoff/mod* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Tersoff/MOD file in the *potentials* directory of the LAMMPS distribution have a ".tersoff.mod" suffix. Potential files for the *tersoff/mod/c* style have the suffix ".tersoff.modc". Lines that are not blank or comments (starting with #) define parameters for a triplet of elements. The parameters in a single entry correspond to coefficients in the formulae above:

- element 1 (the center atom in a 3-body interaction)
- element 2 (the atom bonded to the center atom)
- element 3 (the atom influencing the 1-2 bond in a bond-order sense)
- β
- α
- h
- η
- β_{ters} = 1 (dummy parameter)
- λ_2 (1/distance units)
- B (energy units)
- R (distance units)
- D (distance units)
- λ_1 (1/distance units)
- A (energy units)
- n
- c1
- c2
- c3
- c4
- c5
- c0 (energy units, tersoff/mod/c only):ul

The n, η, λ_2, B, λ_1, and A parameters are only used for two-body interactions. The β, α, c1, c2, c3, c4, c5, h parameters are only used for three-body interactions. The R and D parameters are used for both two-body and three-body interactions. The c0 term applies to *tersoff/mod/c* only. The non-annotated parameters are unitless.

The Tersoff/MOD potential file must contain entries for all the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries.

For a single-element simulation, only a single entry is required (e.g. SiSiSi). As annotated above, the first element in the entry is the center atom in a three-body interaction and it is bonded to the 2nd atom and the bond is influenced by the 3rd atom. Thus an entry for SiSiSi means Si bonded to a Si with another Si atom influencing the bond.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.437.4 Restrictions

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This pair style requires the *newton* setting to be "on" for pair interactions.

The Tersoff/MOD potential files provided with LAMMPS (see the potentials directory) are parameterized for metal *units*. You can use the Tersoff/MOD potential with any LAMMPS units, but you would need to create your own Tersoff/MOD potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

18.437.5 Related commands

pair_coeff

Default: none

(Kumagai) T. Kumagai, S. Izumi, S. Hara, S. Sakai, Comp. Mat. Science, 39, 457 (2007).

(Tersoff_1) J. Tersoff, Phys Rev B, 37, 6991 (1988).

(Tersoff_2) J. Tersoff, Phys Rev B, 38, 9902 (1988).

(Murty) M.V.R. Murty, H.A. Atwater, Phys Rev B, 51, 4889 (1995).

(Schelling) Patrick K. Schelling, Comp. Mat. Science, 44, 274 (2008).

18.438 pair_style tersoff/zbl command

18.439 pair_style tersoff/zbl/gpu command

18.440 pair_style tersoff/zbl/kk command

18.441 pair_style tersoff/zbl/omp command

18.441.1 Syntax

```
pair_style tersoff/zbl
```

18.441.2 Examples

```
pair_style tersoff/zbl
pair_coeff * * SiC.tersoff.zbl Si C Si
```

18.441.3 Description

The *tersoff/zbl* style computes a 3-body Tersoff potential *(Tersoff_1)* with a close-separation pairwise modification based on a Coulomb potential and the Ziegler-Biersack-Littmark universal screening function *(ZBL)*, giving the energy

E of a system of atoms as

$$
\begin{aligned}
E &= \frac{1}{2}\sum_i \sum_{j\neq i} V_{ij} \\
V_{ij} &= (1 - f_F(r_{ij}))V_{ij}^{ZBL} + f_F(r_{ij})V_{ij}^{Tersoff} \\
f_F(r_{ij}) &= \frac{1}{1+e^{-A_F(r_{ij}-r_C)}}
\end{aligned}
$$

$$
\begin{aligned}
V_{ij}^{ZBL} &= \frac{1}{4\pi\epsilon_0}\frac{Z_1 Z_2\, e^2}{r_{ij}}\phi(r_{ij}/a) \\
a &= \frac{0.8854\, a_0}{Z_1^{0.23} + Z_2^{0.23}} \\
\phi(x) &= 0.1818e^{-3.2x} + 0.5099e^{-0.9423x} + 0.2802e^{-0.4029x} + 0.02817e^{-0.2016x}
\end{aligned}
$$

$$
\begin{aligned}
V_{ij}^{Tersoff} &= f_C(r_{ij})\left[f_R(r_{ij}) + b_{ij} f_A(r_{ij})\right] \\
f_C(r) &= \begin{cases} 1 & : \quad r < R - D \\ \frac{1}{2} - \frac{1}{2}\sin\left(\frac{\pi}{2}\frac{r-R}{D}\right) & : \quad R - D < r < R + D \\ 0 & : \quad r > R + D \end{cases} \\
f_R(r) &= A\exp(-\lambda_1 r) \\
f_A(r) &= -B\exp(-\lambda_2 r) \\
b_{ij} &= (1 + \beta^n {\zeta_{ij}}^n)^{-\frac{1}{2n}} \\
\zeta_{ij} &= \sum_{k\neq i,j} f_C(r_{ik}) g(\theta_{ijk}) \exp\left[{\lambda_3}^m (r_{ij} - r_{ik})^m\right] \\
g(\theta) &= \gamma_{ijk}\left(1 + \frac{c^2}{d^2} - \frac{c^2}{[d^2 + (\cos\theta - \cos\theta_0)^2]}\right)
\end{aligned}
$$

The f_F term is a fermi-like function used to smoothly connect the ZBL repulsive potential with the Tersoff potential. There are 2 parameters used to adjust it: A_F and r_C. A_F controls how "sharp" the transition is between the two, and r_C is essentially the cutoff for the ZBL potential.

For the ZBL portion, there are two terms. The first is the Coulomb repulsive term, with Z1, Z2 as the number of protons in each nucleus, e as the electron charge (1 for metal and real units) and ϵ_0 as the permittivity of vacuum. The second part is the ZBL universal screening function, with a0 being the Bohr radius (typically 0.529 Angstroms), and the remainder of the coefficients provided by the original paper. This screening function should be applicable to most systems. However, it is only accurate for small separations (i.e. less than 1 Angstrom).

For the Tersoff portion, f_R is a two-body term and f_A includes three-body interactions. The summations in the formula are over all neighbors J and K of atom I within a cutoff distance = R + D.

Only a single pair_coeff command is used with the *tersoff/zbl* style which specifies a Tersoff/ZBL potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of Tersoff/ZBL elements to atom types

See the *pair_coeff* doc page for alternate ways to specify the path for the potential file.

As an example, imagine the SiC.tersoff.zbl file has Tersoff/ZBL values for Si and C. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * SiC.tersoff Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the Tersoff/ZBL file. The final C argument maps LAMMPS atom type 4 to the C element in the Tersoff/ZBL file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *tersoff/zbl* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Tersoff/ZBL files in the *potentials* directory of the LAMMPS distribution have a ".tersoff.zbl" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements. The parameters in a single entry correspond to coefficients in the formula above:

- element 1 (the center atom in a 3-body interaction)
- element 2 (the atom bonded to the center atom)
- element 3 (the atom influencing the 1-2 bond in a bond-order sense)
- m
- γ
- λ_3 (1/distance units)
- c
- d
- $\cos\theta_0$ (can be a value < -1 or > 1)
- n
- β
- λ_2 (1/distance units)
- B (energy units)
- R (distance units)
- D (distance units)
- λ_1 (1/distance units)
- A (energy units)
- Z_i
- Z_j
- ZBLcut (distance units)
- ZBLexpscale (1/distance units)

The n, β, λ_2, B, λ_1, and A parameters are only used for two-body interactions. The m, γ, λ_3, c, d, and $\cos\theta_0$ parameters are only used for three-body interactions. The R and D parameters are used for both two-body and three-body interactions. The Z_i, Z_j, ZBLcut, ZBLexpscale parameters are used in the ZBL repulsive portion of the potential and in the Fermi-like function. The non-annotated parameters are unitless. The value of m must be 3 or 1.

The Tersoff/ZBL potential file must contain entries for all the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries.

For a single-element simulation, only a single entry is required (e.g. SiSiSi). For a two-element simulation, the file must contain 8 entries (for SiSiSi, SiSiC, SiCSi, SiCC, CSiSi, CSiC, CCSi, CCC), that specify Tersoff parameters for all permutations of the two elements interacting in three-body configurations. Thus for 3 elements, 27 entries would be required, etc.

As annotated above, the first element in the entry is the center atom in a three-body interaction and it is bonded to the 2nd atom and the bond is influenced by the 3rd atom. Thus an entry for SiCC means Si bonded to a C with another C atom influencing the bond. Thus three-body parameters for SiCSi and SiSiC entries will not, in general, be the same. The parameters used for the two-body interaction come from the entry where the 2nd element is repeated. Thus the two-body parameters for Si interacting with C, comes from the SiCC entry.

The parameters used for a particular three-body interaction come from the entry with the corresponding three elements. The parameters used only for two-body interactions (n, β, λ_2, B, λ_1, and A) in entries whose 2nd and 3rd element are different (e.g. SiCSi) are not used for anything and can be set to 0.0 if desired.

Note that the twobody parameters in entries such as SiCC and CSiSi are often the same, due to the common use of symmetric mixing rules, but this is not always the case. For example, the beta and n parameters in Tersoff_2 *(Tersoff_2)* are not symmetric.

We chose the above form so as to enable users to define all commonly used variants of the Tersoff portion of the potential. In particular, our form reduces to the original Tersoff form when m = 3 and gamma = 1, while it reduces to the form of *Albe et al.* when beta = 1 and m = 1. Note that in the current Tersoff implementation in LAMMPS, m must be specified as either 3 or 1. Tersoff used a slightly different but equivalent form for alloys, which we will refer to as Tersoff_2 potential *(Tersoff_2)*.

LAMMPS parameter values for Tersoff_2 can be obtained as follows: $\gamma = \omega_{ijk}$, $\lambda_3 = 0$ and the value of m has no effect. The parameters for species i and j can be calculated using the Tersoff_2 mixing rules:

$$\begin{aligned}
\lambda_1^{i,j} &= \frac{1}{2}(\lambda_1^i + \lambda_1^j) \\
\lambda_2^{i,j} &= \frac{1}{2}(\lambda_2^i + \lambda_2^j) \\
A_{i,j} &= (A_i A_j)^{1/2} \\
B_{i,j} &= \chi_{ij}(B_i B_j)^{1/2} \\
R_{i,j} &= (R_i R_j)^{1/2} \\
S_{i,j} &= (S_i S_j)^{1/2}
\end{aligned}$$

Tersoff_2 parameters R and S must be converted to the LAMMPS parameters R and D (R is different in both forms), using the following relations: R=(R'+S')/2 and D=(S'-R')/2, where the primes indicate the Tersoff_2 parameters.

In the potentials directory, the file SiCGe.tersoff provides the LAMMPS parameters for Tersoff's various versions of Si, as well as his alloy parameters for Si, C, and Ge. This file can be used for pure Si, (three different versions), pure C, pure Ge, binary SiC, and binary SiGe. LAMMPS will generate an error if this file is used with any combination involving C and Ge, since there are no entries for the GeC interactions (Tersoff did not publish parameters for this cross-interaction.) Tersoff files are also provided for the SiC alloy (SiC.tersoff) and the GaN (GaN.tersoff) alloys.

Many thanks to Rutuparna Narulkar, David Farrell, and Xiaowang Zhou for helping clarify how Tersoff parameters for alloys have been defined in various papers. Also thanks to Ram Devanathan for providing the base ZBL implementation.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above from values in the potential file.

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.441.4 Restrictions

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This pair style requires the *newton* setting to be "on" for pair interactions.

The Tersoff/ZBL potential files provided with LAMMPS (see the potentials directory) are parameterized for metal *units*. You can use the Tersoff potential with any LAMMPS units, but you would need to create your own Tersoff potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

18.441.5 Related commands

pair_coeff

Default: none

(Tersoff_1) J. Tersoff, Phys Rev B, 37, 6991 (1988).

(ZBL) J.F. Ziegler, J.P. Biersack, U. Littmark, 'Stopping and Ranges of Ions in Matter' Vol 1, 1985, Pergamon Press.

(Albe) J. Nord, K. Albe, P. Erhart and K. Nordlund, J. Phys.: Condens. Matter, 15, 5649(2003).

(Tersoff_2) J. Tersoff, Phys Rev B, 39, 5566 (1989); errata (PRB 41, 3248)

18.442 pair_style thole command

18.443 pair_style lj/cut/thole/long command

18.444 pair_style lj/cut/thole/long/omp command

18.444.1 Syntax

```
pair_style style args
```

- style = *thole* or *lj/cut/thole/long* or *lj/cut/thole/long/omp*

- args = list of arguments for a particular style

```
thole args = damp cutoff
  damp = global damping parameter
  cutoff = global cutoff (distance units)
lj/cut/thole/long or lj/cut/thole/long/omp args = damp cutoff (cutoff2)
  damp = global damping parameter
  cutoff = global cutoff for LJ (and Thole if only 1 arg) (distance units)
  cutoff2 = global cutoff for Thole (optional) (distance units)
```

18.444.2 Examples

```
pair_style hybrid/overlay ... thole 2.6 12.0
pair_coeff 1 1 thole 1.0
pair_coeff 1 2 thole 1.0 2.6 10.0
pair_coeff * 2 thole 1.0 2.6

pair_style lj/cut/thole/long 2.6 12.0
```

18.444.3 Description

The *thole* pair styles are meant to be used with force fields that include explicit polarization through Drude dipoles. This link describes how to use the *thermalized Drude oscillator model* in LAMMPS and polarizable models in LAMMPS are discussed on the *Howto polarizable* doc page.

The *thole* pair style should be used as a sub-style within in the *pair_style hybrid/overlay* command, in conjunction with a main pair style including Coulomb interactions, i.e. any pair style containing *coul/cut* or *coul/long* in its style name.

The *lj/cut/thole/long* pair style is equivalent to, but more convenient that the frequent combination *hybrid/overlay lj/cut/coul/long cutoff thole damp cutoff*2. It is not only a shorthand for this pair_style combination, but it also allows for mixing pair coefficients instead of listing them all. The *lj/cut/thole/long* pair style is also a bit faster because it avoids an overlay and can benefit from OMP acceleration. Moreover, it uses a more precise approximation of the direct Coulomb interaction at short range similar to *coul/long/cs*, which stabilizes the temperature of Drude particles.

The *thole* pair styles compute the Coulomb interaction damped at short distances by a function

$$T_{ij}(r_{ij}) = 1 - \left(1 + \frac{s_{ij} r_{ij}}{2}\right) \exp\left(-s_{ij} r_{ij}\right)$$

This function results from an adaptation to point charges *(Noskov)* of the dipole screening scheme originally proposed by *Thole*. The scaling coefficient s_{ij} is determined by the polarizability of the atoms, α_i, and by a Thole damping parameter a. This Thole damping parameter usually takes a value of 2.6, but in certain force fields the value can depend upon the atom types. The mixing rule for Thole damping parameters is the arithmetic average, and for polarizabilities the geometric average between the atom-specific values.

$$s_{ij} = \frac{a_{ij}}{(\alpha_{ij})^{1/3}} = \frac{(a_i + a_j)/2}{[(\alpha_i \alpha_j)^{1/2}]^{1/3}}$$

The damping function is only applied to the interactions between the point charges representing the induced dipoles on polarizable sites, that is, charges on Drude particles, $q_{D,i}$, and opposite charges, $-q_{D,i}$, located on the respective core particles (to which each Drude particle is bonded). Therefore, Thole screening is not applied to the full charge of the core particle q_i, but only to the $-q_{D,i}$ part of it.

The interactions between core charges are subject to the weighting factors set by the *special_bonds* command. The interactions between Drude particles and core charges or non-polarizable atoms are also subject to these weighting factors. The Drude particles inherit the 1-2, 1-3 and 1-4 neighbor relations from their respective cores.

For pair_style *thole*, the following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the example above.

- α (distance units^3)
- damp
- cutoff (distance units)

The last two coefficients are optional. If not specified the global Thole damping parameter or global cutoff specified in the pair_style command are used. In order to specify a cutoff (third argument) a damp parameter (second argument) must also be specified.

For pair style *lj/cut/thole/long*, the following coefficients must be defined for each pair of atoms types via the *pair_coeff* command.

- ϵ (energy units)
- σ (length units)
- α (distance units^3)
- damp
- LJ cutoff (distance units)

The last two coefficients are optional and default to the global values from the *pair_style* command line.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing:

The *thole* pair style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

The *lj/cut/thole/long* pair style does support mixing. Mixed coefficients are defined using

$$\alpha_{ij} = \sqrt{\alpha_i \alpha_j}$$

$$a_{ij} = \frac{1}{2}(a_i + a_j)$$

18.444.4 Restrictions

These pair styles are part of the USER-DRUDE package. They are only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This pair_style should currently not be used with the *charmm dihedral style* if the latter has non-zero 1-4 weighting factors. This is because the *thole* pair style does not know which pairs are 1-4 partners of which dihedrals.

The *lj/cut/thole/long* pair style should be used with a *Kspace solver* like PPPM or Ewald, which is only enabled if LAMMPS was built with the kspace package.

18.444.5 Related commands

fix drude, *fix langevin/drude*, *fix drude/transform*, *compute temp/drude pair_style lj/cut/coul/long*

Default: none

(Noskov) Noskov, Lamoureux and Roux, J Phys Chem B, 109, 6705 (2005).

(Thole) Chem Phys, 59, 341 (1981).

18.445 pair_style tri/lj command

18.445.1 Syntax

```
pair_style tri/lj cutoff
```

cutoff = global cutoff for interactions (distance units)

18.445.2 Examples

```
pair_style tri/lj 3.0
pair_coeff * * 1.0 1.0
pair_coeff 1 1 1.0 1.5 2.5
```

18.445.3 Description

Style *tri/lj* treats particles which are triangles as a set of small spherical particles that tile the triangle surface as explained below. Interactions between two triangles, each with N1 and N2 spherical particles, are calculated as the pairwise sum of N1*N2 Lennard-Jones interactions. Interactions between a triangle with N spherical particles and a point particle are treated as the pairwise sum of N Lennard-Jones interactions. See the *pair_style lj/cut* doc page for the definition of Lennard-Jones interactions.

The cutoff distance for an interaction between 2 triangles, or between a triangle and a point particle, is calculated from the position of the triangle (its centroid), not between pairs of individual spheres comprising the triangle. Thus an interaction is either calculated in its entirety or not at all.

The set of non-overlapping spherical particles that represent a triangle, for purposes of this pair style, are generated in the following manner. Assume the triangle is of type I, and sigma_II has been specified. We want a set of spheres with centers in the plane of the triangle, none of them larger in diameter than sigma_II, which completely cover the triangle's area, but with minimal overlap and a minimal total number of spheres. This is done in a recursive manner.

Place a sphere at the centroid of the original triangle. Calculate what diameter it must have to just cover all 3 corner points of the triangle. If that diameter is equal to or smaller than sigma_II, then include a sphere of the calculated diameter in the set of covering spheres. It the diameter is larger than sigma_II, then split the triangle into 2 triangles by bisecting its longest side. Repeat the process on each sub-triangle, recursing as far as needed to generate a set of covering spheres. When finished, the original criteria are met, and the set of covering spheres should be near minimal in number and overlap, at least for input triangles with a reasonable aspect-ratio.

The LJ interaction between 2 spheres on different triangles of types I,J is computed with an arithmetic mixing of the sigma values of the 2 spheres and using the specified epsilon value for I,J atom types. Note that because the sigma values for triangles spheres is computed using only sigma_II values, specific to the triangles's type, this means that any specified sigma_IJ values (for I != J) are effectively ignored.

For style *tri/lj*, the following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- epsilon (energy units)
- sigma (distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global cutoff is used.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of this pair style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style does not write its information to *binary restart files*.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.445.4 Restrictions

This style is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

Defining particles to be triangles so they participate in tri/tri or tri/particle interactions requires the use the *atom_style tri* command.

18.445.5 Related commands

pair_coeff, *pair_style line/lj*

Default: none

18.446 pair_style ufm command

18.447 pair_style ufm/gpu command

18.448 pair_style ufm/omp command

18.449 pair_style ufm/opt command

18.449.1 Syntax

```
pair_style ufm cutoff
```

- cutoff = global cutoff for *ufm* interactions (distance units)

18.449.2 Examples

```
pair_style ufm 4.0
pair_coeff 1 1 100.0 1.0 2.5
pair_coeff * * 100.0 1.0

pair_style ufm 4.0
pair_coeff * * 10.0 1.0
variable prefactor equal ramp(10,100)
fix 1 all adapt 1 pair ufm epsilon * * v_prefactor
```

18.449.3 Description

Style *ufm* computes pairwise interactions using the Uhlenbeck-Ford model (UFM) potential *(Paula Leite2016)* which is given by

$$E = -\varepsilon \ln\left[1 - \exp\left(-r^2/\sigma^2\right)\right] \qquad r < r_c$$
$$\varepsilon = p\, k_B\, T$$

where r_c is the cutoff, σ is a distance-scale and ϵ is an energy-scale, i.e., a product of Boltzmann constant k_B, temperature T and the Uhlenbeck-Ford p-parameter which is responsible to control the softness of the interactions *(Paula Leite2017)*. This model is useful as a reference system for fluid-phase free-energy calculations *(Paula Leite2016)*.

The following coefficients must be defined for each pair of atom types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- ϵ (energy units)
- σ (distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global *ufm* cutoff is used.

The *fix adapt* command can be used to vary epsilon and sigma for this pair style over the course of a simulation, in which case pair_coeff settings for epsilon and sigma must still be specified, but will be overridden. For example these

commands will vary the prefactor epsilon for all pairwise interactions from 10.0 at the beginning to 100.0 at the end of a run:

```
variable prefactor equal ramp(10,100)
fix 1 all adapt 1 pair ufm epsilon * * v_prefactor
```

Note: The thermodynamic integration procedure can be performed with this potential using *fix adapt*. This command will rescale the force on each atom by varying a scale variable, which always starts with value 1.0. The syntax is the same described above, however, changing epsilon to scale. A detailed explanation of how to use this command and perform nonequilibrium thermodynamic integration in LAMMPS is given in the paper by *(Freitas)*.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the A coefficient and cutoff distance for this pair style can be mixed. A is always mixed via a *geometric* rule. The cutoff is mixed according to the pair_modify mix value. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style support the *pair_modify* shift option for the energy of the pair interaction.

The *pair_modify* table and tail are not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.449.4 Restrictions

none

18.449.5 Related commands

pair_coeff, *fix adapt*

Default: none

(Paula Leite2017) Paula Leite, Santos-Florez, and de Koning, Phys Rev E, 96, 32115 (2017).

(Paula Leite2016) Paula Leite , Freitas, Azevedo, and de Koning, J Chem Phys, 126, 044509 (2016).

(Freitas) Freitas, Asta, and de Koning, Computational Materials Science, 112, 333 (2016).

18.450 pair_style vashishta command

18.451 pair_style vashishta/gpu command

18.452 pair_style vashishta/omp command

18.453 pair_style vashishta/kk command

18.454 pair_style vashishta/table command

18.455 pair_style vashishta/table/omp command

18.455.1 Syntax

```
pair_style style args
```

- style = *vashishta* or *vashishta/table* or *vashishta/omp* or *vashishta/table/omp*
- args = list of arguments for a particular style

```
vashishta or vashishta/omp args = none
vashishta/table or vashishta/table/omp args = Ntable cutinner
  Ntable = # of tabulation points
  cutinner = tablulate from cutinner to cutoff
```

18.455.2 Examples

```
pair_style vashishta
pair_coeff * * SiC.vashishta Si C

pair_style vashishta/table 100000 0.2
pair_coeff * * SiC.vashishta Si C
```

18.455.3 Description

The *vashishta* and *vashishta/table* styles compute the combined 2-body and 3-body family of potentials developed in the group of Priya Vashishta and collaborators. By combining repulsive, screened Coulombic, screened charge-dipole, and dispersion interactions with a bond-angle energy based on the Stillinger-Weber potential, this potential has been used to describe a variety of inorganic compounds, including SiO2 *Vashishta1990*, SiC *Vashishta2007*, and InP *Branicio2009*.

The potential for the energy U of a system of atoms is

$$U = \sum_i^N \sum_{j>i}^N U_{ij}^{(2)}(r_{ij}) + \sum_i^N \sum_{j\neq i}^N \sum_{k>j,k\neq i}^N U_{ijk}^{(3)}(r_{ij}, r_{ik}, \theta_{ijk})$$

$$U_{ij}^{(2)}(r) = \frac{H_{ij}}{r^{\eta_{ij}}} + \frac{Z_i Z_j}{r}\exp(-r/\lambda_{1,ij}) - \frac{D_{ij}}{r^4}\exp(-r/\lambda_{4,ij}) - \frac{W_{ij}}{r^6}, r < r_{c,ij}$$

$$U_{ijk}^{(3)}(r_{ij}, r_{ik}, \theta_{ijk}) = B_{ijk}\frac{\left[\cos\theta_{ijk} - \cos\theta_{0ijk}\right]^2}{1 + C_{ijk}\left[\cos\theta_{ijk} - \cos\theta_{0ijk}\right]^2} \times$$

$$\exp\left(\frac{\gamma_{ij}}{r_{ij} - r_{0,ij}}\right)\exp\left(\frac{\gamma_{ik}}{r_{ik} - r_{0,ik}}\right), r_{ij} < r_{0,ij}, r_{ik} < r_{0,ik}$$

where we follow the notation used in *Branicio2009*. U^2 is a two-body term and U3 is a three-body term. The summation over two-body terms is over all neighbors J within a cutoff distance = r_c. The twobody terms are shifted and tilted by a linear function so that the energy and force are both zero at r_c. The summation over three-body terms is over all neighbors *i* and *k* within a cut-off distance $= r_0$, where the exponential screening function becomes zero.

The *vashishta* style computes these formulas analytically. The *vashishta/table* style tabulates the analytic values for *Ntable* points from cutinner to the cutoff of the potential. The points are equally spaced in R^2 space from cutinner^2 to cutoff^2. For the two-body term in the above equation, a linear interpolation for each pairwise distance between adjacent points in the table. In practice the tabulated version can run 3-5x faster than the analytic version with moderate to little loss of accuracy for Ntable values between 10000 and 1000000. It is not recommended to use less than 5000 tabulation points.

Only a single pair_coeff command is used with either style which specifies a Vashishta potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of Vashishta elements to atom types

See the *pair_coeff* doc page for alternate ways to specify the path for the potential file.

As an example, imagine a file SiC.vashishta has parameters for Si and C. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * SiC.vashishta Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the file. The final C argument maps LAMMPS atom type 4 to the C element in the file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *vashishta* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Vashishta files in the *potentials* directory of the LAMMPS distribution have a ".vashishta" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements. The parameters in a single entry correspond to the two-body and three-body coefficients in the formulae above:

- element 1 (the center atom in a 3-body interaction)

- element 2
- element 3
- H (energy units)
- η
- Z_i (electron charge units)
- Z_j (electron charge units)
- λ_1 (distance units)
- D (energy units)
- λ_4 (distance units)
- W (energy units)
- r_c (distance units)
- B (energy units)
- γ
- r_0 (distance units)
- C
- $\cos\theta_0$

The non-annotated parameters are unitless. The Vashishta potential file must contain entries for all the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries. For a single-element simulation, only a single entry is required (e.g. SiSiSi). For a two-element simulation, the file must contain 8 entries (for SiSiSi, SiSiC, SiCSi, SiCC, CSiSi, CSiC, CCSi, CCC), that specify parameters for all permutations of the two elements interacting in three-body configurations. Thus for 3 elements, 27 entries would be required, etc.

Depending on the particular version of the Vashishta potential, the values of these parameters may be keyed to the identities of zero, one, two, or three elements. In order to make the input file format unambiguous, general, and simple to code, LAMMPS uses a slightly confusing method for specifying parameters. All parameters are divided into two classes: two-body and three-body. Two-body and three-body parameters are handled differently, as described below. The two-body parameters are H, η, λ_1, D, λ_4, W, r_c, γ, and r_0. They appear in the above formulae with two subscripts. The parameters Z_i and Z_j are also classified as two-body parameters, even though they only have 1 subscript. The three-body parameters are B, C, $\cos\theta_0$. They appear in the above formulae with three subscripts. Two-body and three-body parameters are handled differently, as described below.

The first element in each entry is the center atom in a three-body interaction, while the second and third elements are two neighbor atoms. Three-body parameters for a central atom I and two neighbors J and K are taken from the IJK entry. Note that even though three-body parameters do not depend on the order of J and K, LAMMPS stores three-body parameters for both IJK and IKJ. The user must ensure that these values are equal. Two-body parameters for an atom I interacting with atom J are taken from the IJJ entry, where the 2nd and 3rd elements are the same. Thus the two-body parameters for Si interacting with C come from the SiCC entry. Note that even though two-body parameters (except possibly gamma and r0 in U3) do not depend on the order of the two elements, LAMMPS will get the Si-C value from the SiCC entry and the C-Si value from the CSiSi entry. The user must ensure that these values are equal. Two-body parameters appearing in entries where the 2nd and 3rd elements are different are stored but never used. It is good practice to enter zero for these values. Note that the three-body function U3 above contains the two-body parameters γ and r_0. So U3 for a central C atom bonded to an Si atom and a second C atom will take three-body parameters from the CSiC entry, but two-body parameters from the CCC and CSiSi entries.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above from values in the potential file.

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style does not write its information to *binary restart files*, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.455.4 Restrictions

These pair style are part of the MANYBODY package. They is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

These pair styles requires the *newton* setting to be "on" for pair interactions.

The Vashishta potential files provided with LAMMPS (see the potentials directory) are parameterized for metal *units*. You can use the Vashishta potential with any LAMMPS units, but you would need to create your own potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

18.455.5 Related commands

pair_coeff

Default: none

(Vashishta1990) P. Vashishta, R. K. Kalia, J. P. Rino, Phys. Rev. B 41, 12197 (1990).

(Vashishta2007) P. Vashishta, R. K. Kalia, A. Nakano, J. P. Rino. J. Appl. Phys. 101, 103515 (2007).

(Branicio2009) Branicio, Rino, Gan and Tsuzuki, J. Phys Condensed Matter 21 (2009) 095002

18.456 pair_style yukawa command

18.457 pair_style yukawa/gpu command

18.458 pair_style yukawa/omp command

18.459 pair_style yukawa/kk command

18.459.1 Syntax

```
pair_style yukawa kappa cutoff
```

- kappa = screening length (inverse distance units)
- cutoff = global cutoff for Yukawa interactions (distance units)

18.459.2 Examples

```
pair_style yukawa 2.0 2.5
pair_coeff 1 1 100.0 2.3
pair_coeff * * 100.0
```

18.459.3 Description

Style *yukawa* computes pairwise interactions with the formula

$$E = A\frac{e^{-\kappa r}}{r} \qquad r < r_c$$

r_c is the cutoff.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- A (energy*distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global yukawa cutoff is used.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the A coefficient and cutoff distance for this pair style can be mixed. A is an energy value mixed like a LJ epsilon. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style supports the *pair_modify* shift option for the energy of the pair interaction.

The *pair_modify* table option is not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.459.4 Restrictions

none

18.459.5 Related commands

pair_coeff

Default: none

18.460 pair_style yukawa/colloid command

18.461 pair_style yukawa/colloid/gpu command

18.462 pair_style yukawa/colloid/omp command

18.462.1 Syntax

```
pair_style yukawa/colloid kappa cutoff
```

- kappa = screening length (inverse distance units)
- cutoff = global cutoff for colloidal Yukawa interactions (distance units)

18.462.2 Examples

```
pair_style yukawa/colloid 2.0 2.5
pair_coeff 1 1 100.0 2.3
pair_coeff * * 100.0
```

18.462.3 Description

Style *yukawa/colloid* computes pairwise interactions with the formula

$$E = \frac{A}{\kappa} e^{-\kappa(r-(r_i+r_j))} \qquad r < r_c$$

where r_i and r_j are the radii of the two particles and r_c is the cutoff.

In contrast to *pair_style yukawa*, this functional form arises from the Coulombic interaction between two colloid particles, screened due to the presence of an electrolyte, see the book by *Safran* for a derivation in the context of DLVO theory. *Pair_style yukawa* is a screened Coulombic potential between two point-charges and uses no such approximation.

This potential applies to nearby particle pairs for which the Derjagin approximation holds, meaning $h << r_i + r_j$, where *h* is the surface-to-surface separation of the two particles.

When used in combination with *pair_style colloid*, the two terms become the so-called DLVO potential, which combines electrostatic repulsion and van der Waals attraction.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- A (energy/distance units)
- cutoff (distance units)

The prefactor A is determined from the relationship between surface charge and surface potential due to the presence of electrolyte. Note that the A for this potential style has different units than the A used in *pair_style yukawa*. For low surface potentials, i.e. less than about 25 mV, A can be written as:

$$A = 2\pi R \varepsilon \varepsilon_0 \kappa \psi^2$$

where

- *R* = colloid radius (distance units)
- ε_0 = permittivity of free space (charge^2/energy/distance units)
- ε = relative permittivity of fluid medium (dimensionless)
- κ = inverse screening length (1/distance units)
- ψ = surface potential (energy/charge units)

The last coefficient is optional. If not specified, the global yukawa/colloid cutoff is used.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the A coefficient and cutoff distance for this pair style can be mixed. A is an energy value mixed like a LJ epsilon. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style supports the *pair_modify* shift option for the energy of the pair interaction.

The *pair_modify* table option is not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.462.4 Restrictions

This style is part of the COLLOID package. It is only enabled if LAMMPS was built with that package. See the *Build package* doc page for more info.

This pair style requires that atoms be finite-size spheres with a diameter, as defined by the *atom_style sphere* command.

Per-particle polydispersity is not yet supported by this pair style; per-type polydispersity is allowed. This means all particles of the same type must have the same diameter. Each type can have a different diameter.

18.462.5 Related commands

pair_coeff

Default: none

(Safran) Safran, Statistical Thermodynamics of Surfaces, Interfaces, And Membranes, Westview Press, ISBN: 978-0813340791 (2003).

18.463 pair_style zbl command

18.464 pair_style zbl/gpu command

18.465 pair_style zbl/kk command

18.466 pair_style zbl/omp command

18.466.1 Syntax

```
pair_style zbl inner outer
```

- inner = distance where switching function begins
- outer = global cutoff for ZBL interaction

18.466.2 Examples

```
pair_style zbl 3.0 4.0
pair_coeff * * 73.0 73.0
pair_coeff 1 1 14.0 14.0
```

18.466.3 Description

Style *zbl* computes the Ziegler-Biersack-Littmark (ZBL) screened nuclear repulsion for describing high-energy collisions between atoms. *(Ziegler)*. It includes an additional switching function that ramps the energy, force, and curvature smoothly to zero between an inner and outer cutoff. The potential energy due to a pair of atoms at a distance r_ij is given by:

$$E_{ij}^{ZBL} = \frac{1}{4\pi\epsilon_0}\frac{Z_i Z_j\, e^2}{r_{ij}}\phi(r_{ij}/a) + S(r_{ij})$$
$$a = \frac{0.46850}{Z_i^{0.23} + Z_j^{0.23}}$$
$$\phi(x) = 0.18175e^{-3.19980x} + 0.50986e^{-0.94229x} + 0.28022e^{-0.40290x} + 0.02817e^{-0.20162x}$$

where *e* is the electron charge, ϵ_0 is the electrical permittivity of vacuum, and Z_i and Z_j are the nuclear charges of the two atoms. The switching function $S(r)$ is identical to that used by *pair_style lj/gromacs*. Here, the inner and outer cutoff are the same for all pairs of atom types.

The following coefficients must be defined for each pair of atom types via the *pair_coeff* command as in the examples above, or in the LAMMPS data file.

- Z_i (atomic number for first atom type, e.g. 13.0 for aluminum)
- Z_j (ditto for second atom type)

The values of Z_i and Z_j are normally equal to the atomic numbers of the two atom types. Thus, the user may optionally specify only the coefficients for each $i == i$ pair, and rely on the obvious mixing rule for cross interactions (see below). Note that when $i == i$ it is required that $Z_i == Z_j$. When used with *hybrid/overlay* and pairs are assigned to more than one sub-style, the mixing rule is not used and each pair of types interacting with the ZBL sub-style must be included in a pair_coeff command.

Note: The numerical values of the exponential decay constants in the screening function depend on the unit of distance. In the above equation they are given for units of angstroms. LAMMPS will automatically convert these values to the distance unit of the specified LAMMPS *units* setting. The values of Z should always be given as multiples of a proton's charge, e.g. 29.0 for copper.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs *i,j* and $i \neq i$, the Z_i and Z_j coefficients can be mixed by taking Z_i and Z_j from the values specified for $i == i$ and $j == j$ cases. When used with *hybrid/overlay* and pairs are assigned to more than one sub-style, the mixing rule is not used and each pair of types interacting with the ZBL sub-style must be included in a pair_coeff command. The *pair_modify* mix option has no effect on the mixing behavior

The ZBL pair style does not support the *pair_modify* shift option, since the ZBL interaction is already smoothed to 0.0 at the cutoff.

The *pair_modify* table option is not relevant for this pair style.

This pair style does not support the *pair_modify* tail option for adding long-range tail corrections to energy and pressure, since there are no corrections for a potential that goes to 0.0 at the cutoff.

This pair style does not write information to *binary restart files*, so pair_style and pair_coeff commands must be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner*, *middle*, *outer* keywords.

18.466.4 Restrictions

none

18.466.5 Related commands

pair_coeff

Default: none

(Ziegler) J.F. Ziegler, J. P. Biersack and U. Littmark, "The Stopping and Range of Ions in Matter," Volume 1, Pergamon, 1985.

18.467 pair_style zero command

18.467.1 Syntax

```
pair_style zero cutoff [nocoeff]
```

- zero = style name of this pair style
- cutoff = global cutoff (distance units)
- nocoeff = ignore all pair_coeff parameters (optional)

18.467.2 Examples

```
pair_style zero 10.0
pair_style zero 5.0 nocoeff
pair_coeff * *
pair_coeff 1 2*4 3.0
```

18.467.3 Description

Define a global or per-type cutoff length for the purpose of building a neighbor list and acquiring ghost atoms, but do not compute any pairwise forces or energies.

This can be useful for fixes or computes which require a neighbor list to enumerate pairs of atoms within some cutoff distance, but when pairwise forces are not otherwise needed. Examples are the *fix bond/create*, *compute rdf*, *compute voronoi/atom* commands.

Note that the *comm_modify cutoff* command can be used to insure communication of ghost atoms even when a pair style is not defined, but it will not trigger neighbor list generation.

The optional *nocoeff* flag allows to read data files with a PairCoeff section for any pair style. Similarly, any pair_coeff commands will only be checked for the atom type numbers and the rest ignored. In this case, only the global cutoff will be used.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- cutoff (distance units)

This coefficient is optional. If not specified, the global cutoff specified in the pair_style command is used. If the pair_style has been specified with the optional *nocoeff* flag, then a cutoff pair coefficient is ignored.

Mixing, shift, table, tail correction, restart, rRESPA info:

The cutoff distance for this pair style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style writes its information to *binary restart files*, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style supports the use of the *inner*, *middle*, and *outer* keywords of the *run_style respa* command.

18.467.4 Restrictions

none

18.467.5 Related commands

pair_style none

Default: none

CHAPTER

NINETEEN

BOND STYLES

19.1 bond_style class2 command

19.2 bond_style class2/omp command

19.3 bond_style class2/kk command

19.3.1 Syntax

```
bond_style class2
```

19.3.2 Examples

```
bond_style class2
bond_coeff 1 1.0 100.0 80.0 80.0
```

19.3.3 Description

The *class2* bond style uses the potential

$$E = K_2(r - r_0)^2 + K_3(r - r_0)^3 + K_4(r - r_0)^4$$

where r_0 is the equilibrium bond distance.

See *(Sun)* for a description of the COMPASS class2 force field.

The following coefficients must be defined for each bond type via the *bond_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- r_0 (distance)
- K_2 (energy/distance^2)
- K_3 (energy/distance^3)
- K_4 (energy/distance^4)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

19.3.4 Restrictions

This bond style can only be used if LAMMPS was built with the CLASS2 package. See the *Build package* doc page for more info.

19.3.5 Related commands

bond_coeff, *delete_bonds*

Default: none

(Sun) Sun, J Phys Chem B 102, 7338-7364 (1998).

19.4 bond_style fene command

19.5 bond_style fene/intel command

19.6 bond_style fene/kk command

19.7 bond_style fene/omp command

19.7.1 Syntax

```
bond_style fene
```

19.7.2 Examples

```
bond_style fene
bond_coeff 1 30.0 1.5 1.0 1.0
```

19.7.3 Description

The *fene* bond style uses the potential

$$E = -0.5KR_0^2 \ln\left[1 - \left(\frac{r}{R_0}\right)^2\right] + 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right] + \epsilon$$

to define a finite extensible nonlinear elastic (FENE) potential *(Kremer)*, used for bead-spring polymer models. The first term is attractive, the 2nd Lennard-Jones term is repulsive. The first term extends to R_0, the maximum extent of the bond. The 2nd term is cutoff at $2^{\frac{1}{6}}\sigma$, the minimum of the LJ potential.

The following coefficients must be defined for each bond type via the *bond_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy/distance^2)
- R_0 (distance)
- ϵ (energy)
- σ (distance)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

19.7.4 Restrictions

This bond style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

You typically should specify *special_bonds fene* or *special_bonds lj/coul 0 1 1* to use this bond style. LAMMPS will issue a warning it that's not the case.

19.7.5 Related commands

bond_coeff, *delete_bonds*

Default: none

(Kremer) Kremer, Grest, J Chem Phys, 92, 5057 (1990).

19.8 bond_style fene/expand command

19.9 bond_style fene/expand/omp command

19.9.1 Syntax

```
bond_style fene/expand
```

19.9.2 Examples

```
bond_style fene/expand
bond_coeff 1 30.0 1.5 1.0 1.0 0.5
```

19.9.3 Description

The *fene/expand* bond style uses the potential

$$E = -0.5KR_0^2 \ln\left[1 - \left(\frac{(r-\Delta)}{R_0}\right)^2\right] + 4\epsilon\left[\left(\frac{\sigma}{(r-\Delta)}\right)^{12} - \left(\frac{\sigma}{(r-\Delta)}\right)^{6}\right] + \epsilon$$

to define a finite extensible nonlinear elastic (FENE) potential *(Kremer)*, used for bead-spring polymer models. The first term is attractive, the 2nd Lennard-Jones term is repulsive.

The *fene/expand* bond style is similar to *fene* except that an extra shift factor of Δ (positive or negative) is added to r to effectively change the bead size of the bonded atoms. The first term now extends to $R_0 + \Delta$ and the 2nd term is cutoff at $2^{\frac{1}{6}}\sigma + \Delta$.

The following coefficients must be defined for each bond type via the *bond_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy/distance^2)
- R_0 (distance)
- ϵ (energy)
- σ (distance)
- Δ (distance)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

19.9.4 Restrictions

This bond style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

You typically should specify *special_bonds fene* or *special_bonds lj/coul 0 1 1* to use this bond style. LAMMPS will issue a warning it that's not the case.

19.9.5 Related commands

bond_coeff, *delete_bonds*

Default: none

(Kremer) Kremer, Grest, J Chem Phys, 92, 5057 (1990).

19.10 bond_style gromos command

19.11 bond_style gromos/omp command

19.11.1 Syntax

```
bond_style gromos
```

19.11.2 Examples

```
bond_style gromos
bond_coeff 5 80.0 1.2
```

19.11.3 Description

The *gromos* bond style uses the potential

$$E = K(r^2 - r_0^2)^2$$

where r_0 is the equilibrium bond distance. Note that the usual 1/4 factor is included in K.

The following coefficients must be defined for each bond type via the *bond_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy/distance^4)
- r_0 (distance)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

19.11.4 Restrictions

This bond style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

19.11.5 Related commands

bond_coeff, *delete_bonds*

Default: none

19.12 bond_style harmonic command

19.13 bond_style harmonic/intel command

19.14 bond_style harmonic/kk command

19.15 bond_style harmonic/omp command

19.15.1 Syntax

```
bond_style harmonic
```

19.15.2 Examples

```
bond_style harmonic
bond_coeff 5 80.0 1.2
```

19.15.3 Description

The *harmonic* bond style uses the potential

$$E = K(r - r_0)^2$$

where r_0 is the equilibrium bond distance. Note that the usual 1/2 factor is included in K.

The following coefficients must be defined for each bond type via the *bond_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy/distance^2)
- r_0 (distance)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

19.15.4 Restrictions

This bond style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

19.15.5 Related commands

bond_coeff, *delete_bonds*

Default: none

19.16 bond_style harmonic/shift command

19.17 bond_style harmonic/shift/omp command

19.17.1 Syntax

```
bond_style harmonic/shift
```

19.17.2 Examples

```
bond_style harmonic/shift
bond_coeff 5 10.0 0.5 1.0
```

19.17.3 Description

The *harmonic/shift* bond style is a shifted harmonic bond that uses the potential

$$E = \frac{U_{\text{min}}}{(r_0 - r_c)^2} \left[(r - r_0)^2 - (r_c - r_0)^2 \right]$$

where r_0 is the equilibrium bond distance, and r_c the critical distance. The potential is $-U_{\text{min}}$ at $r0$ and zero at r_c. The spring constant is $k = U_{\text{min}}/[2(r_0 - r_c)^2]$.

The following coefficients must be defined for each bond type via the *bond_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- U_{min} (energy)
- r_0 (distance)
- r_c (distance)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

19.17.4 Restrictions

This bond style can only be used if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

19.17.5 Related commands

bond_coeff, *delete_bonds*, *bond_harmonic*

Default: none

19.18 bond_style harmonic/shift/cut command

19.19 bond_style harmonic/shift/cut/omp command

19.19.1 Syntax

```
bond_style harmonic/shift/cut
```

19.19.2 Examples

```
bond_style harmonic/shift/cut
bond_coeff 5 10.0 0.5 1.0
```

19.19.3 Description

The *harmonic/shift/cut* bond style is a shifted harmonic bond that uses the potential

$$E = \frac{U_{\text{min}}}{(r_0 - r_c)^2} \left[(r - r_0)^2 - (r_c - r_0)^2 \right]$$

where r_0 is the equilibrium bond distance, and rc the critical distance. The bond potential is zero for distances $r > r_c$. The potential is $-U_{\text{min}}$ at r_0 and zero at r_c. The spring constant is $k = U_{\text{min}}/[2(r_0 - r_c)^2]$.

The following coefficients must be defined for each bond type via the *bond_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- U_{min} (energy)
- r_0 (distance)
- r_c (distance)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

19.19.4 Restrictions

This bond style can only be used if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

19.19.5 Related commands

bond_coeff, *delete_bonds*, *bond_harmonic*, *bond_style harmonic/shift*

Default: none

19.20 bond_style hybrid command

19.20.1 Syntax

```
bond_style hybrid style1 style2 ...
```

- style1,style2 = list of one or more bond styles

19.20.2 Examples

19.20.3 Description

The *hybrid* style enables the use of multiple bond styles in one simulation. A bond style is assigned to each bond type. For example, bonds in a polymer flow (of bond type 1) could be computed with a *fene* potential and bonds in the wall boundary (of bond type 2) could be computed with a *harmonic* potential. The assignment of bond type to style is made via the *bond_coeff* command or in the data file.

In the bond_coeff commands, the name of a bond style must be added after the bond type, with the remaining coefficients being those appropriate to that style. In the example above, the 2 bond_coeff commands set bonds of bond type 1 to be computed with a *harmonic* potential with coefficients 80.0, 1.2 for K, r_0. All other bond types (2-N) are computed with a *fene* potential with coefficients 30.0, 1.5, 1.0, 1.0 for K, R_0, ϵ, σ.

If bond coefficients are specified in the data file read via the *read_data* command, then the same rule applies. E.g. "harmonic" or "fene" must be added after the bond type, for each line in the "Bond Coeffs" section, e.g.

```
Bond Coeffs

1 harmonic 80.0 1.2
2 fene 30.0 1.5 1.0 1.0
...
```

A bond style of *none* with no additional coefficients can be used in place of a bond style, either in a input script bond_coeff command or in the data file, if you desire to turn off interactions for specific bond types.

19.20.4 Restrictions

This bond style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

Unlike other bond styles, the hybrid bond style does not store bond coefficient info for individual sub-styles in a *binary restart files*. Thus when restarting a simulation from a restart file, you need to re-specify bond_coeff commands.

19.20.5 Related commands

bond_coeff, *delete_bonds*

Default: none

19.21 bond_style mm3 command

19.21.1 Syntax

```
bond_style mm3
```

19.21.2 Examples

```
bond_style mm3
bond_coeff 1 100.0 107.0
```

19.21.3 Description

The *mm3* bond style uses the potential that is anharmonic in the bond as defined in *(Allinger)*

$$E = K(r - r_0)^2 \left[1 - 2.55(r - r_0) + (7/12)2.55^2(r - r_0)^2\right]$$

where r_0 is the equilibrium value of the bond, and K is a prefactor. The anharmonic prefactors have units angstrom^(-n): -2.55 angstrom^(-1) and (7/12)2.55^2 angstrom^(-2). The code takes care of the necessary unit conversion for these factors internally. Note that the MM3 papers contains an error in Eq (1): (7/12)2.55 should be replaced with (7/12)2.55^2

The following coefficients must be defined for each bond type via the *bond_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy/distance^2)
- r_0 (distance)

19.21.4 Restrictions

This bond style can only be used if LAMMPS was built with the USER_YAFF package. See the *Build package* doc page for more info.

19.21.5 Related commands

bond_coeff

Default: none

(Allinger) Allinger, Yuh, Lii, JACS, 111(23), 8551-8566 (1989),

19.22 bond_style morse command

19.23 bond_style morse/omp command

19.23.1 Syntax

```
bond_style morse
```

19.23.2 Examples

```
bond_style morse
bond_coeff 5 1.0 2.0 1.2
```

19.23.3 Description

The *morse* bond style uses the potential

$$E = D\left[1 - e^{-\alpha(r-r_0)}\right]^2$$

where r_0 is the equilibrium bond distance, α is a stiffness parameter, and D determines the depth of the potential well.

The following coefficients must be defined for each bond type via the *bond_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- D (energy)
- α (inverse distance)
- r_0 (distance)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

19.23.4 Restrictions

This bond style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

19.23.5 Related commands

bond_coeff, *delete_bonds*

Default: none

19.24 bond_style none command

19.24.1 Syntax

```
bond_style none
```

19.24.2 Examples

```
bond_style none
```

19.24.3 Description

Using a bond style of none means bond forces and energies are not computed, even if pairs of bonded atoms were listed in the data file read by the *read_data* command.

See the *bond_style zero* command for a way to calculate bond statistics, but compute no bond interactions.

19.24.4 Restrictions

none

Related commands: none

bond_style zero

Default: none

19.25 bond_style nonlinear command

19.26 bond_style nonlinear/omp command

19.26.1 Syntax

```
bond_style nonlinear
```

19.26.2 Examples

```
bond_style nonlinear
bond_coeff 2 100.0 1.1 1.4
```

19.26.3 Description

The *nonlinear* bond style uses the potential

$$E = \frac{\epsilon(r - r_0)^2}{[\lambda^2 - (r - r_0)^2]}$$

to define an anharmonic spring *(Rector)* of equilibrium length r_0 and maximum extension lamda.

The following coefficients must be defined for each bond type via the *bond_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- ϵ (energy)
- r_0 (distance)
- λ (distance)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

19.26.4 Restrictions

This bond style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

19.26.5 Related commands

bond_coeff, *delete_bonds*

Default: none

(Rector) Rector, Van Swol, Henderson, Molecular Physics, 82, 1009 (1994).

19.27 bond_style oxdna/fene command

19.28 bond_style oxdna2/fene command

19.29 bond_style oxrna2/fene command

19.29.1 Syntax

```
bond_style oxdna/fene

bond_style oxdna2/fene

bond_style oxrna2/fene
```

19.29.2 Examples

```
bond_style oxdna/fene
bond_coeff * 2.0 0.25 0.7525

bond_style oxdna2/fene
bond_coeff * 2.0 0.25 0.7564

bond_style oxrna2/fene
bond_coeff \* 2.0 0.25 0.76107
```

19.29.3 Description

The *oxdna/fene* , *oxdna2/fene* and *oxrna2/fene* bond styles use the potential

$$E = -\frac{\epsilon}{2} \ln \left[1 - \left(\frac{r - r_0}{\Delta} \right)^2 \right]$$

to define a modified finite extensible nonlinear elastic (FENE) potential *(Ouldridge)* to model the connectivity of the phosphate backbone in the oxDNA/oxRNA force field for coarse-grained modelling of DNA/RNA.

The following coefficients must be defined for the bond type via the *bond_coeff* command as given in the above example, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- ϵ (energy)
- Δ (distance)
- r_0 (distance)

Note: The oxDNA bond style has to be used together with the corresponding oxDNA pair styles for excluded volume interaction *oxdna/excv* , stacking *oxdna/stk* , cross-stacking *oxdna/xstk* and coaxial stacking interaction *oxdna/coaxstk* as well as hydrogen-bonding interaction *oxdna/hbond* (see also documentation of *pair_style oxdna/excv*). For the oxDNA2 *(Snodin)* bond style the analogous pair styles *oxdna2/excv* , *oxdna2/stk* , *oxdna2/xstk* , *oxdna2/coaxstk* , *oxdna2/hbond* and an additional Debye-Hueckel pair style *oxdna2/dh* have to be defined. The same applies to the oxRNA2 *(Sulc1)* styles. The coefficients in the above example have to be kept fixed and cannot be changed without reparameterizing the entire model.

Example input and data files for DNA and RNA duplexes can be found in examples/USER/cgdna/examples/oxDNA/ , /oxDNA2/ and /oxRNA2/. A simple python setup tool which creates single straight or helical DNA strands, DNA/RNA duplexes or arrays of DNA/RNA duplexes can be found in examples/USER/cgdna/util/.

Please cite *(Henrich)* in any publication that uses this implementation. The article contains general information on the model, its implementation and performance as well as the structure of the data and input file. The preprint version of the article can be found here. Please cite also the relevant oxDNA/oxRNA publications. These are *(Ouldridge)* and *(Ouldridge-DPhil)* for oxDNA, *(Snodin)* for oxDNA2, *(Sulc1)* for oxRNA2 and for sequence-specific hydrogen-bonding and stacking interactions *(Sulc2)*.

19.29.4 Restrictions

This bond style can only be used if LAMMPS was built with the USER-CGDNA package and the MOLECULE and ASPHERE package. See the *Build package* doc page for more info.

19.29.5 Related commands

pair_style oxdna/excv, *pair_style oxdna2/excv*, *pair_style oxrna2/excv*, *bond_coeff* , *fix nve/dotc/langevin*

Default:

none

(Henrich) O. Henrich, Y. A. Gutierrez-Fosado, T. Curk, T. E. Ouldridge, Eur. Phys. J. E 41, 57 (2018).

(Ouldridge-DPhil) T.E. Ouldridge, Coarse-grained modelling of DNA and DNA self-assembly, DPhil. University of Oxford (2011).

(Ouldridge) T.E. Ouldridge, A.A. Louis, J.P.K. Doye, J. Chem. Phys. 134, 085101 (2011).

(Snodin) B.E. Snodin, F. Randisi, M. Mosayebi, et al., J. Chem. Phys. 142, 234901 (2015).

(Sulc1) P. Sulc, F. Romano, T. E. Ouldridge, et al., J. Chem. Phys. 140, 235102 (2014).

(Sulc2) P. Sulc, F. Romano, T.E. Ouldridge, L. Rovigatti, J.P.K. Doye, A.A. Louis, J. Chem. Phys. 137, 135101 (2012).

19.30 bond_style quartic command

19.31 bond_style quartic/omp command

19.31.1 Syntax

```
bond_style quartic
```

19.31.2 Examples

```
bond_style quartic
bond_coeff 2 1200 -0.55 0.25 1.3 34.6878
```

19.31.3 Description

The *quartic* bond style uses the potential

$$E = K(r - R_c)^2(r - R_c - B_1)(r - R_c - B_2) + U_0 + 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] + \epsilon$$

to define a bond that can be broken as the simulation proceeds (e.g. due to a polymer being stretched). The σ and ϵ used in the LJ portion of the formula are both set equal to 1.0 by LAMMPS.

The following coefficients must be defined for each bond type via the *bond_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy/distance^4)
- B_1 (distance)
- B_2 (distance)
- R_c (distance)
- U_0 (energy)

This potential was constructed to mimic the FENE bond potential for coarse-grained polymer chains. When monomers with $\sigma = \epsilon = 1.0$ are used, the following choice of parameters gives a quartic potential that looks nearly like the FENE

potential:

$$
\begin{aligned}
K &= 1200 \\
B_1 &= -0.55 \\
B_2 &= 0.25 \\
R_c &= 1.3 \\
U_0 &= 34.6878
\end{aligned}
$$

Different parameters can be specified using the *bond_coeff* command, but you will need to choose them carefully so they form a suitable bond potential.

R_c is the cutoff length at which the bond potential goes smoothly to a local maximum. If a bond length ever becomes $> R_c$, LAMMPS "breaks" the bond, which means two things. First, the bond potential is turned off by setting its type to 0, and is no longer computed. Second, a pairwise interaction between the two atoms is turned on, since they are no longer bonded.

LAMMPS does the second task via a computational sleight-of-hand. It subtracts the pairwise interaction as part of the bond computation. When the bond breaks, the subtraction stops. For this to work, the pairwise interaction must always be computed by the *pair_style* command, whether the bond is broken or not. This means that *special_bonds* must be set to 1,1,1, as indicated as a restriction below.

Note that when bonds are dumped to a file via the *dump local* command, bonds with type 0 are not included. The *delete_bonds* command can also be used to query the status of broken bonds or permanently delete them, e.g.:

```
delete_bonds all stats
delete_bonds all bond 0 remove
```

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

19.31.4 Restrictions

This bond style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

The *quartic* style requires that *special_bonds* parameters be set to 1,1,1. Three- and four-body interactions (angle, dihedral, etc) cannot be used with *quartic* bonds.

19.31.5 Related commands

bond_coeff, *delete_bonds*

Default: none

19.32 bond_style table command

19.33 bond_style table/omp command

19.33.1 Syntax

```
bond_style table style N
```

- style = *linear* or *spline* = method of interpolation
- N = use N values in table

19.33.2 Examples

```
bond_style table linear 1000
bond_coeff 1 file.table ENTRY1
```

19.33.3 Description

Style *table* creates interpolation tables of length *N* from bond potential and force values listed in a file(s) as a function of bond length. The files are read by the *bond_coeff* command.

The interpolation tables are created by fitting cubic splines to the file values and interpolating energy and force values at each of *N* distances. During a simulation, these tables are used to interpolate energy and force values as needed. The interpolation is done in one of 2 styles: *linear* or *spline*.

For the *linear* style, the bond length is used to find 2 surrounding table values from which an energy or force is computed by linear interpolation.

For the *spline* style, a cubic spline coefficients are computed and stored at each of the *N* values in the table. The bond length is used to find the appropriate set of coefficients which are used to evaluate a cubic polynomial which computes the energy or force.

The following coefficients must be defined for each bond type via the *bond_coeff* command as in the example above.

- filename
- keyword

The filename specifies a file containing tabulated energy and force values. The keyword specifies a section of the file. The format of this file is described below.

The format of a tabulated file is as follows (without the parenthesized comments):

```
# Bond potential for harmonic (one or more comment or blank lines)

HAM                             (keyword is the first text on line)
N 101 FP 0 0 EQ 0.5             (N, FP, EQ  parameters)
                                (blank line)
1 0.00 338.0000 1352.0000       (index, bond-length, energy, force)
2 0.01 324.6152 1324.9600
...
101 1.00 338.0000 -1352.0000
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the *bond_coeff* command. The next line lists (in any order) one or more parameters for the table. Each parameter is a keyword followed by one or more numeric values.

The parameter "N" is required and its value is the number of table entries that follow. Note that this may be different than the *N* specified in the *bond_style table* command. Let Ntable = *N* in the bond_style command, and Nfile = "N" in the tabulated file. What LAMMPS does is a preliminary interpolation by creating splines using the Nfile tabulated values as nodal points. It uses these to interpolate as needed to generate energy and force values at Ntable different points. The resulting tables of length Ntable are then used as described above, when computing energy and force for individual bond lengths. This means that if you want the interpolation tables of length Ntable to match exactly what is in the tabulated file (with effectively no preliminary interpolation), you should set Ntable = Nfile.

The "FP" parameter is optional. If used, it is followed by two values fplo and fphi, which are the derivatives of the force at the innermost and outermost bond lengths. These values are needed by the spline construction routines. If not specified by the "FP" parameter, they are estimated (less accurately) by the first two and last two force values in the table.

The "EQ" parameter is also optional. If used, it is followed by a the equilibrium bond length, which is used, for example, by the *fix shake* command. If not used, the equilibrium bond length is to the distance in the table with the lowest potential energy.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is the bond length r (in distance units), the 3rd value is the energy (in energy units), and the 4th is the force (in force units). The bond lengths must range from a LO value to a HI value, and increase from one line to the next. If the actual bond length is ever smaller than the LO value or larger than the HI value, then the calculation is aborted with an error, so it is advisable to cover the whole range of possible bond lengths.

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart info:

This bond style writes the settings for the "bond_style table" command to *binary restart files*, so a bond_style command does not need to specified in an input script that reads a restart file. However, the coefficient information is not stored in the restart file, since it is tabulated in the potential files. Thus, bond_coeff commands do need to be specified in the restart input script.

19.33.4 Restrictions

This bond style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

19.33.5 Related commands

bond_coeff, *delete_bonds*

Default: none

19.34 bond_style zero command

19.34.1 Syntax

```
bond_style zero [nocoeff]
```

19.34.2 Examples

```
bond_style zero
bond_style zero nocoeff
bond_coeff *
bond_coeff * 2.14
```

19.34.3 Description

Using an bond style of zero means bond forces and energies are not computed, but the geometry of bond pairs is still accessible to other commands.

As an example, the *compute bond/local* command can be used to compute distances for the list of pairs of bond atoms listed in the data file read by the *read_data* command. If no bond style is defined, this command cannot be used.

The optional *nocoeff* flag allows to read data files with a BondCoeff section for any bond style. Similarly, any bond_coeff commands will only be checked for the bond type number and the rest ignored.

Note that the *bond_coeff* command must be used for all bond types. If specified, there can be only one value, which is going to be used to assign an equilibrium distance, e.g. for use with *fix shake*.

19.34.4 Restrictions

none

19.34.5 Related commands

bond_style none

Default: none

CHAPTER

TWENTY

ANGLE STYLES

20.1 angle_style charmm command

20.2 angle_style charmm/intel command

20.3 angle_style charmm/kk command

20.4 angle_style charmm/omp command

20.4.1 Syntax

```
angle_style charmm
```

20.4.2 Examples

```
angle_style charmm
angle_coeff 1 300.0 107.0 50.0 3.0
```

20.4.3 Description

The *charmm* angle style uses the potential

$$E = K(\theta - \theta_0)^2 + K_{ub}(r - r_{ub})^2$$

with an additional Urey_Bradley term based on the distance r between the 1st and 3rd atoms in the angle. K, θ_0, K_{ub}, and R_{ub} are coefficients defined for each angle type.

See *(MacKerell)* for a description of the CHARMM force field.

The following coefficients must be defined for each angle type via the *angle_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy/radian^2)
- θ_0 (degrees)
- K_{ub} (energy/distance^2)
- r_{ub} (distance)

θ_0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of K are in energy/radian^2.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

20.4.4 Restrictions

This angle style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

20.4.5 Related commands

angle_coeff

Default: none

(MacKerell) MacKerell, Bashford, Bellott, Dunbrack, Evanseck, Field, Fischer, Gao, Guo, Ha, et al, J Phys Chem, 102, 3586 (1998).

20.5 angle_style class2 command

20.6 angle_style class2/kk command

20.7 angle_style class2/omp command

20.8 angle_style class2/p6 command

20.8.1 Syntax

```
angle_style class2
```

20.8.2 Examples

```
angle_style class2
angle_coeff * 75.0
angle_coeff 1 bb 10.5872 1.0119 1.5228
angle_coeff * ba 3.6551 24.895 1.0119 1.5228
```

20.8.3 Description

The *class2* angle style uses the potential

$$
\begin{aligned}
E &= E_a + E_{bb} + E_{ba} \\
E_a &= K_2(\theta - \theta_0)^2 + K_3(\theta - \theta_0)^3 + K_4(\theta - \theta_0)^4 \\
E_{bb} &= M(r_{ij} - r_1)(r_{jk} - r_2) \\
E_{ba} &= N_1(r_{ij} - r_1)(\theta - \theta_0) + N_2(r_{jk} - r_2)(\theta - \theta_0)
\end{aligned}
$$

where E_a is the angle term, E_{bb} is a bond-bond term, and E_{ba} is a bond-angle term. θ_0 is the equilibrium angle and r_1 and r_2 are the equilibrium bond lengths.

See *(Sun)* for a description of the COMPASS class2 force field.

Coefficients for the E_a, E_{bb}, and E_{ba} formulas must be defined for each angle type via the *angle_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands.

These are the 4 coefficients for the E_a formula:

- θ_0 (degrees)
- K_2 (energy/radian^2)
- K_3 (energy/radian^3)
- K_4 (energy/radian^4)

θ_0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of the various K are in per-radian.

For the E_{bb} formula, each line in a *angle_coeff* command in the input script lists 4 coefficients, the first of which is "bb" to indicate they are BondBond coefficients. In a data file, these coefficients should be listed under a "BondBond Coeffs" heading and you must leave out the "bb", i.e. only list 3 coefficients after the angle type.

- bb
- M (energy/distance^2)
- r_1 (distance)
- r_2 (distance)

For the E_{ba} formula, each line in a *angle_coeff* command in the input script lists 5 coefficients, the first of which is "ba" to indicate they are BondAngle coefficients. In a data file, these coefficients should be listed under a "BondAngle Coeffs" heading and you must leave out the "ba", i.e. only list 4 coefficients after the angle type.

- ba
- N_1 (energy/distance^2)
- N_2 (energy/distance^2)
- r_1 (distance)
- r_2 (distance)

The θ_0 value in the E_{ba} formula is not specified, since it is the same value from the E_a formula.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

The *class2/p6* angle style uses the *class2* potential expanded to sixth order:

$$E_a = K_2 (\theta - \theta_0)^2 + K_3 (\theta - \theta_0)^3 + K_4 (\theta - \theta_0)^4 + K_5 (\theta - \theta_0)^5 + K_6 (\theta - \theta_0)^6$$

In this expanded term 6 coefficients for the E_a formula need to be set:

- θ_0 (degrees)
- K_2 (energy/radian^2)
- K_3 (energy/radian^3)
- K_4 (energy/radian^4)
- K_5 (energy/radian^5)
- K_6 (energy/radian^6)

The bond-bond and bond-angle terms remain unchanged.

20.8.4 Restrictions

This angle style can only be used if LAMMPS was built with the CLASS2 package. For the *class2/p6* style LAMMPS needs to be built with the USER-MOFFF package. See the *Build package* doc page for more info.

20.8.5 Related commands

angle_coeff

Default: none

(Sun) Sun, J Phys Chem B 102, 7338-7364 (1998).

20.9 angle_style cosine command

20.10 angle_style cosine/omp command

20.11 angle_style cosine/kk command

20.11.1 Syntax

```
angle_style cosine
```

20.11.2 Examples

```
angle_style cosine
angle_coeff * 75.0
```

20.11.3 Description

The *cosine* angle style uses the potential

$$E = K[1 + \cos(\theta)]$$

where K is defined for each angle type.

The following coefficients must be defined for each angle type via the *angle_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

20.11.4 Restrictions

This angle style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

20.11.5 Related commands

angle_coeff

Default: none

20.12 angle_style cosine/buck6d command

20.12.1 Syntax

```
angle_style cosine/buck6d
```

20.12.2 Examples

```
angle_style cosine/buck6d
angle_coeff 1  cosine/buck6d  1.978350  4  180.000000
```

20.12.3 Description

The *cosine/buck6d* angle style uses the potential

$$E = K\left[1 + \cos(n\theta - \theta_0)\right]$$

where K is the energy constant, n is the periodic multiplicity and θ_0 is the equilibrium angle.

The coefficients must be defined for each angle type via the *angle_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands in the following order:

- K (energy)
- n
- θ_0 (degrees)

θ_0 is specified in degrees, but LAMMPS converts it to radians internally.

Additional to the cosine term the *cosine/buck6d* angle style computes the short range (vdW) interaction belonging to the *pair_style buck6d* between the end atoms of the angle. For this reason this angle style only works in combination with the *pair_style buck6d* styles and needs the *special_bonds* 1-3 interactions to be weighted 0.0 to prevent double counting.

20.12.4 Restrictions

cosine/buck6d can only be used in combination with the *pair_style buck6d* style and with a *special_bonds* 0.0 weighting of 1-3 interactions.

This angle style can only be used if LAMMPS was built with the USER-MOFFF package. See the *Build package* doc page for more info.

20.12.5 Related commands

angle_coeff

Default: none

20.13 angle_style cosine/delta command

20.14 angle_style cosine/delta/omp command

20.14.1 Syntax

```
angle_style cosine/delta
```

20.14.2 Examples

```
angle_style cosine/delta
angle_coeff 2*4 75.0 100.0
```

20.14.3 Description

The *cosine/delta* angle style uses the potential

$$E = K[1 - \cos(\theta - \theta_0)]$$

where θ_0 is the equilibrium value of the angle, and K is a prefactor. Note that the usual 1/2 factor is included in K.

The following coefficients must be defined for each angle type via the *angle_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- θ_0 (degrees)

θ_0 is specified in degrees, but LAMMPS converts it to radians internally.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

20.14.4 Restrictions

This angle style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

20.14.5 Related commands

angle_coeff, *angle_style cosine/squared*

Default: none

20.15 angle_style cosine/periodic command

20.16 angle_style cosine/periodic/omp command

20.16.1 Syntax

```
angle_style cosine/periodic
```

20.16.2 Examples

```
angle_style cosine/periodic
angle_coeff * 75.0 1 6
```

20.16.3 Description

The *cosine/periodic* angle style uses the following potential, which is commonly used in the *DREIDING* force field, particularly for organometallic systems where n = 4 might be used for an octahedral complex and n = 3 might be used for a trigonal center:

$$E = C\left[1 - B(-1)^n \cos\left(n\theta\right)\right]$$

where C, B and n are coefficients defined for each angle type.

See *(Mayo)* for a description of the DREIDING force field

The following coefficients must be defined for each angle type via the *angle_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- C (energy)

- B = 1 or -1
- n = 1, 2, 3, 4, 5 or 6 for periodicity

Note that the prefactor C is specified and not the overall force constant $K = \frac{C}{n^2}$. When $B = 1$, it leads to a minimum for the linear geometry. When $B = -1$, it leads to a maximum for the linear geometry.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

20.16.4 Restrictions

This angle style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

20.16.5 Related commands

angle_coeff

Default: none

(Mayo) Mayo, Olfason, Goddard III, J Phys Chem, 94, 8897-8909 (1990).

20.17 angle_style cosine/shift command

20.18 angle_style cosine/shift/omp command

20.18.1 Syntax

```
angle_style cosine/shift
```

20.18.2 Examples

```
angle_style cosine/shift
angle_coeff * 10.0 45.0
```

20.18.3 Description

The *cosine/shift* angle style uses the potential

$$E = -\frac{U_{\text{min}}}{2}\left[1 + \cos(\theta - \theta_0)\right]$$

where θ_0 is the equilibrium angle. The potential is bounded between $-U_{\text{min}}$ and zero. In the neighborhood of the minimum $E = -U_{\text{min}} + U_{\text{min}}/4(\theta - \theta_0)^2$ hence the spring constant is $\frac{U_{\text{min}}}{2}$.

The following coefficients must be defined for each angle type via the *angle_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- U_{min} (energy)
- θ (angle)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

20.18.4 Restrictions

This angle style can only be used if LAMMPS was built with the USER-MISC package.

20.18.5 Related commands

angle_coeff, *angle_style cosine/shift/exp*

Default: none

20.19 angle_style cosine/shift/exp command

20.20 angle_style cosine/shift/exp/omp command

20.20.1 Syntax

```
angle_style cosine/shift/exp
```

20.20.2 Examples

```
angle_style cosine/shift/exp
angle_coeff * 10.0 45.0 2.0
```

20.20.3 Description

The *cosine/shift/exp* angle style uses the potential

$$E = -U_{\text{min}} \frac{e^{-aU(\theta,\theta_0)} - 1}{e^a - 1} \quad \text{with} \quad U(\theta,\theta_0) = -0.5\,(1 + \cos(\theta - \theta_0))$$

where U_{min}, θ, and a are defined for each angle type.

The potential is bounded between $[-U_{\text{min}}, 0]$ and the minimum is located at the angle θ_0. The a parameter can be both positive or negative and is used to control the spring constant at the equilibrium.

The spring constant is given by $k = A\exp(A)U_{\text{min}}/[2(\exp(a) - 1)]$. For $a > 3$, $\frac{k}{U_{\text{min}}} = \frac{a}{2}$ to better than 5% relative error. For negative values of the a parameter, the spring constant is essentially zero, and anharmonic terms takes over. The potential is furthermore well behaved in the limit $a \to 0$, where it has been implemented to linear order in a for $a < 0.001$. In this limit the potential reduces to the cosineshifted potential.

The following coefficients must be defined for each angle type via the *angle_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- U_min (energy)
- θ (angle)
- A (real number)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

20.20.4 Restrictions

This angle style can only be used if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

20.20.5 Related commands

angle_coeff, *angle_style cosine/shift*, *dihedral_style cosine/shift/exp*

Default: none

20.21 angle_style cosine/squared command

20.22 angle_style cosine/squared/omp command

20.22.1 Syntax

```
angle_style cosine/squared
```

20.22.2 Examples

```
angle_style cosine/squared
angle_coeff 2*4 75.0 100.0
```

20.22.3 Description

The *cosine/squared* angle style uses the potential

$$E = K[\cos(\theta) - \cos(\theta_0)]^2$$

where θ_0 is the equilibrium value of the angle, and K is a prefactor. Note that the usual 1/2 factor is included in K.

The following coefficients must be defined for each angle type via the *angle_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- θ_0 (degrees)

θ_0 is specified in degrees, but LAMMPS converts it to radians internally.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

20.22.4 Restrictions

This angle style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

20.22.5 Related commands

angle_coeff

Default: none

20.23 angle_style cross command

20.23.1 Syntax

```
angle_style cross
```

20.23.2 Examples

```
angle_style cross
angle_coeff 1 200.0 100.0 100.0 1.25 1.25 107.0
```

20.23.3 Description

The *cross* angle style uses a potential that couples the bond stretches of a bend with the angle stretch of that bend:

$$E = K_{SS}\left(r_{12} - r_{12,0}\right)\left(r_{32} - r_{32,0}\right) + K_{BS0}\left(r_{12} - r_{12,0}\right)\left(\theta - \theta_0\right) + K_{BS1}\left(r_{32} - r_{32,0}\right)\left(\theta - \theta_0\right)$$

where $r_{12,0}$ is the rest value of the bond length between atom 1 and 2, $r_{32,0}$ is the rest value of the bond length between atom 3 and 2, and θ_0 is the rest value of the angle. K_{SS} is the force constant of the bond stretch-bond stretch term and K_{BS0} and K_{BS1} are the force constants of the bond stretch-angle stretch terms.

The following coefficients must be defined for each angle type via the *angle_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K_{SS} (energy/distance^2)
- K_{BS0} (energy/distance/rad)
- K_{BS1} (energy/distance/rad)
- $r_{12,0}$ (distance)
- $r_{32,0}$ (distance)

- θ_0 (degrees)

θ_0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of K_{BS0} and K_{BS1} are in energy/distance/radian.

20.23.4 Restrictions

This angle style can only be used if LAMMPS was built with the USER_YAFF package. See the *Build package* doc page for more info.

20.23.5 Related commands

angle_coeff

Default: none

20.24 angle_style dipole command

20.25 angle_style dipole/omp command

20.25.1 Syntax

```
angle_style dipole
```

20.25.2 Examples

```
angle_style dipole
angle_coeff 6 2.1 180.0
```

20.25.3 Description

The *dipole* angle style is used to control the orientation of a dipolar atom within a molecule *(Orsi)*. Specifically, the *dipole* angle style restrains the orientation of a point dipole μ_j (embedded in atom j) with respect to a reference (bond) vector $\vec{r_{ij}} = \vec{r_i} - \vec{r_j}$, where i is another atom of the same molecule (typically, i and j are also covalently bonded).

It is convenient to define an angle gamma between the 'free' vector $\vec{\mu_j}$ and the reference (bond) vector $\vec{r_{ij}}$:

$$\cos\gamma = \frac{\vec{\mu_j} \cdot \vec{r_{ij}}}{\mu_j \, r_{ij}}$$

The *dipole* angle style uses the potential:

$$E = K(\cos\gamma - \cos\gamma_0)^2$$

where K is a rigidity constant and gamma0 is an equilibrium (reference) angle.

The torque on the dipole can be obtained by differentiating the potential using the 'chain rule' as in appendix C.3 of *(Allen)*:

$$\vec{T_j} = \frac{2K(\cos\gamma - \cos\gamma_0)}{\mu_j \, r_{ij}} \, \vec{r_{ij}} \times \vec{\mu_j}$$

Example: if γ_0 is set to 0 degrees, the torque generated by the potential will tend to align the dipole along the reference direction defined by the (bond) vector $\vec{r_{ij}}$ (in other words, $\vec{\mu_j}$ is restrained to point towards atom i).

The dipolar torque $\vec{T_j}$ must be counterbalanced in order to conserve the local angular momentum. This is achieved via an additional force couple generating a torque equivalent to the opposite of $\vec{T_j}$:

$$-\vec{T_j} = \vec{r_{ij}} \times \vec{F_i}$$
$$\vec{F_j} = -\vec{F_i}$$

where $\vec{F_i}$ and $\vec{F_j}$ are applied on atoms i and j, respectively.

The following coefficients must be defined for each angle type via the *angle_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- γ_0 (degrees)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

20.25.4 Restrictions

This angle style can only be used if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

Note: In the "Angles" section of the data file, the atom ID j defining the direction of the dipole vector to restrain must come before the atom ID of the reference atom i. A third atom ID k must also be provided to comply with the requirement of a valid angle definition. This atom ID k should be chosen to be that of an atom bonded to atom i to avoid errors with "lost angle atoms" when running in parallel. Since the LAMMPS code checks for valid angle definitions, cannot use the same atom ID of either i or j (this was allowed and recommended with older LAMMPS versions).

The *newton* command for intramolecular interactions must be "on" (which is the default except when using some accelerator packages).

This angle style should not be used with SHAKE.

20.25.5 Related commands

angle_coeff, *angle_hybrid*

Default: none

(Orsi) Orsi & Essex, The ELBA force field for coarse-grain modeling of lipid membranes, PloS ONE 6(12): e28637, 2011.

(Allen) Allen & Tildesley, Computer Simulation of Liquids, Clarendon Press, Oxford, 1987.

20.26 angle_style fourier command

20.27 angle_style fourier/omp command

20.27.1 Syntax

```
angle_style fourier
```

20.27.2 Examples

```
angle_style fourier
angle_coeff 75.0 1.0 1.0 1.0
```

20.27.3 Description

The *fourier* angle style uses the potential

$$E = K[C_0 + C_1 \cos(\theta) + C_2 \cos(2\theta)]$$

The following coefficients must be defined for each angle type via the *angle_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- C_0 (real)
- C_1 (real)
- C_2 (real)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

20.27.4 Restrictions

This angle style can only be used if LAMMPS was built with the USER_MISC package. See the *Build package* doc page for more info.

20.27.5 Related commands

angle_coeff

Default: none

20.28 angle_style fourier/simple command

20.29 angle_style fourier/simple/omp command

20.29.1 Syntax

```
angle_style fourier/simple
```

20.29.2 Examples

```
angle_style fourier/simple
angle_coeff 100.0 -1.0 1.0
```

20.29.3 Description

The *fourier/simple* angle style uses the potential

$$E = K[1.0 + c\cos(n\theta)]$$

The following coefficients must be defined for each angle type via the *angle_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- c (real)
- n (real)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

20.29.4 Restrictions

This angle style can only be used if LAMMPS was built with the USER_MISC package. See the *Build package* doc page for more info.

20.29.5 Related commands

angle_coeff

Default: none

20.30 angle_style harmonic command

20.31 angle_style harmonic/intel command

20.32 angle_style harmonic/kk command

20.33 angle_style harmonic/omp command

20.33.1 Syntax

```
angle_style harmonic
```

20.33.2 Examples

```
angle_style harmonic
angle_coeff 1 300.0 107.0
```

20.33.3 Description

The *harmonic* angle style uses the potential

$$E = K(\theta - \theta_0)^2$$

where θ_0 is the equilibrium value of the angle, and K is a prefactor. Note that the usual 1/2 factor is included in K.

The following coefficients must be defined for each angle type via the *angle_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy/radian^2)
- θ_0 (degrees)

θ_0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of K are in energy/radian^2.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

20.33.4 Restrictions

This angle style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

20.33.5 Related commands

angle_coeff

Default: none

20.34 angle_style hybrid command

20.34.1 Syntax

```
angle_style hybrid style1 style2 ...
```

- style1,style2 = list of one or more angle styles

20.34.2 Examples

```
angle_style hybrid harmonic cosine
angle_coeff 1 harmonic 80.0 30.0
angle_coeff 2* cosine 50.0
```

20.34.3 Description

The *hybrid* style enables the use of multiple angle styles in one simulation. An angle style is assigned to each angle type. For example, angles in a polymer flow (of angle type 1) could be computed with a *harmonic* potential and angles in the wall boundary (of angle type 2) could be computed with a *cosine* potential. The assignment of angle type to style is made via the *angle_coeff* command or in the data file.

In the *angle_coeff* commands, the name of an angle style must be added after the angle type, with the remaining coefficients being those appropriate to that style. In the example above, the 2 angle_coeff commands set angles of angle type 1 to be computed with a *harmonic* potential with coefficients 80.0, 30.0 for K, θ_0. All other angle types $(2 - N)$ are computed with a *cosine* potential with coefficient 50.0 for K.

If angle coefficients are specified in the data file read via the *read_data* command, then the same rule applies. E.g. "harmonic" or "cosine", must be added after the angle type, for each line in the "Angle Coeffs" section, e.g.

```
Angle Coeffs

1 harmonic 80.0 30.0
2 cosine 50.0
...
```

If *class2* is one of the angle hybrid styles, the same rule holds for specifying additional BondBond (and BondAngle) coefficients either via the input script or in the data file. I.e. *class2* must be added to each line after the angle type. For lines in the BondBond (or BondAngle) section of the data file for angle types that are not *class2*, you must use an angle style of *skip* as a placeholder, e.g.

```
BondBond Coeffs

1 skip
2 class2 3.6512 1.0119 1.0119
...
```

Note that it is not necessary to use the angle style *skip* in the input script, since BondBond (or BondAngle) coefficients need not be specified at all for angle types that are not *class2*.

An angle style of *none* with no additional coefficients can be used in place of an angle style, either in a input script *angle_coeff* command or in the data file, if you desire to turn off interactions for specific angle types.

20.34.4 Restrictions

This angle style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

Unlike other angle styles, the hybrid angle style does not store angle coefficient info for individual sub-styles in a *binary restart files*. Thus when restarting a simulation from a restart file, you need to re-specify *angle_coeff* commands.

20.34.5 Related commands

angle_coeff

Default: none

20.35 angle_style mm3 command

20.35.1 Syntax

```
angle_style mm3
```

20.35.2 Examples

```
angle_style mm3
angle_coeff 1 100.0 107.0
```

20.35.3 Description

The *mm3* angle style uses the potential that is anharmonic in the angle as defined in *(Allinger)*

$$E = K(\theta - \theta_0)^2 \left[1 - 0.014(\theta - \theta_0) + 5.6(10)^{-5}(\theta - \theta_0)^2 - 7.0(10)^{-7}(\theta - \theta_0)^3 + 9(10)^{-10}(\theta - \theta_0)^4\right]$$

where θ_0 is the equilibrium value of the angle, and K is a prefactor. The anharmonic prefactors have units $\deg^{-n}$, for example $-0.014\,\deg^{-1}$, $5.6 \cdot 10^{-5}\,\deg^{-2}, \ldots$

The following coefficients must be defined for each angle type via the *angle_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy/radian^2)
- θ_0 (degrees)

θ_0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of K are in energy/radian^2.

20.35.4 Restrictions

This angle style can only be used if LAMMPS was built with the USER_YAFF package. See the *Build package* doc page for more info.

20.35.5 Related commands

angle_coeff

Default: none

20.36 angle_style none command

20.36.1 Syntax

```
angle_style none
```

20.36.2 Examples

```
angle_style none
```

20.36.3 Description

Using an angle style of none means angle forces and energies are not computed, even if triplets of angle atoms were listed in the data file read by the *read_data* command.

See the *angle_style zero* command for a way to calculate angle statistics, but compute no angle interactions.

20.36.4 Restrictions

none

20.36.5 Related commands

angle_style zero

Default: none

20.37 angle_style quartic command

20.38 angle_style quartic/omp command

20.38.1 Syntax

```
angle_style quartic
```

20.38.2 Examples

```
angle_style quartic
angle_coeff 1 129.1948 56.8726 -25.9442 -14.2221
```

20.38.3 Description

The *quartic* angle style uses the potential

$$E = K_2(\theta - \theta_0)^2 + K_3(\theta - \theta_0)^3 + K_4(\theta - \theta_0)^4$$

where θ_0 is the equilibrium value of the angle, and K is a prefactor. Note that the usual 1/2 factor is included in K.

The following coefficients must be defined for each angle type via the *angle_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- θ_0 (degrees)
- K_2 (energy/radian^2)
- K_3 (energy/radian^3)
- K_4 (energy/radian^4)

θ_0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of K are in energy/radian^2.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

20.38.4 Restrictions

This angle style can only be used if LAMMPS was built with the USER_MISC package. See the *Build package* doc page for more info.

20.38.5 Related commands

angle_coeff

Default: none

20.39 angle_style sdk command

20.40 angle_style sdk/omp command

20.40.1 Syntax

```
angle_style sdk

angle_style sdk/omp
```

20.40.2 Examples

```
angle_style sdk
angle_coeff 1 300.0 107.0
```

20.40.3 Description

The *sdk* angle style is a combination of the harmonic angle potential,

$$E = K(\theta - \theta_0)^2$$

where θ_0 is the equilibrium value of the angle and K a prefactor, with the *repulsive* part of the non-bonded *lj/sdk* pair style between the atoms 1 and 3. This angle potential is intended for coarse grained MD simulations with the CMM parameterization using the *pair_style lj/sdk*. Relative to the pair_style *lj/sdk*, however, the energy is shifted by ϵ, to avoid sudden jumps. Note that the usual 1/2 factor is included in K.

The following coefficients must be defined for each angle type via the *angle_coeff* command as in the example above:

- K (energy/radian^2)
- θ_0 (degrees)

θ_0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of K are in energy/radian^2. The also required *lj/sdk* parameters will be extracted automatically from the pair_style.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages*

doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

20.40.4 Restrictions

This angle style can only be used if LAMMPS was built with the USER-CGSDK package. See the *Build package* doc page for more info.

20.40.5 Related commands

angle_coeff, *angle_style harmonic*, *pair_style lj/sdk*, *pair_style lj/sdk/coul/long*

Default: none

20.41 angle_style table command

20.42 angle_style table/omp command

20.42.1 Syntax

```
angle_style table style N
```

- style = *linear* or *spline* = method of interpolation
- N = use N values in table

20.42.2 Examples

```
angle_style table linear 1000
angle_coeff 3 file.table ENTRY1
```

20.42.3 Description

Style *table* creates interpolation tables of length *N* from angle potential and derivative values listed in a file(s) as a function of angle The files are read by the *angle_coeff* command.

The interpolation tables are created by fitting cubic splines to the file values and interpolating energy and derivative values at each of *N* angles. During a simulation, these tables are used to interpolate energy and force values on individual atoms as needed. The interpolation is done in one of 2 styles: *linear* or *spline*.

For the *linear* style, the angle is used to find 2 surrounding table values from which an energy or its derivative is computed by linear interpolation.

For the *spline* style, a cubic spline coefficients are computed and stored at each of the *N* values in the table. The angle is used to find the appropriate set of coefficients which are used to evaluate a cubic polynomial which computes the energy or derivative.

The following coefficients must be defined for each angle type via the *angle_coeff* command as in the example above.

- filename
- keyword

The filename specifies a file containing tabulated energy and derivative values. The keyword specifies a section of the file. The format of this file is described below.

The format of a tabulated file is as follows (without the parenthesized comments):

```
# Angle potential for harmonic (one or more comment or blank lines)

HAM                             (keyword is the first text on line)
N 181 FP 0 0 EQ 90.0            (N, FP, EQ parameters)
                                (blank line)
N 181 FP 0 0                    (N, FP parameters)
1 0.0 200.5 2.5                 (index, angle, energy, derivative)
2 1.0 198.0 2.5
...
181 180.0 0.0 0.0
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the *angle_coeff* command. The next line lists (in any order) one or more parameters for the table. Each parameter is a keyword followed by one or more numeric values.

The parameter "N" is required and its value is the number of table entries that follow. Note that this may be different than the *N* specified in the *angle_style table* command. Let Ntable = *N* in the angle_style command, and Nfile = "N" in the tabulated file. What LAMMPS does is a preliminary interpolation by creating splines using the Nfile tabulated values as nodal points. It uses these to interpolate as needed to generate energy and derivative values at Ntable different points. The resulting tables of length Ntable are then used as described above, when computing energy and force for individual angles and their atoms. This means that if you want the interpolation tables of length Ntable to match exactly what is in the tabulated file (with effectively no preliminary interpolation), you should set Ntable = Nfile.

The "FP" parameter is optional. If used, it is followed by two values fplo and fphi, which are the 2nd derivatives at the innermost and outermost angle settings. These values are needed by the spline construction routines. If not specified by the "FP" parameter, they are estimated (less accurately) by the first two and last two derivative values in the table.

The "EQ" parameter is also optional. If used, it is followed by a the equilibrium angle value, which is used, for example, by the *fix shake* command. If not used, the equilibrium angle is set to 180.0.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is the angle value (in degrees), the 3rd value is the energy (in energy units), and the 4th is -dE/d(theta) (also in energy units). The 3rd term is the energy of the 3-atom configuration for the specified angle. The last term is the derivative of the energy with respect to the angle (in degrees, not radians). Thus the units of the last term are still energy, not force. The angle values must increase from one line to the next. The angle values must also begin with 0.0 and end with 180.0, i.e. span the full range of possible angles.

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart info:

This angle style writes the settings for the "angle_style table" command to *binary restart files*, so a angle_style command does not need to specified in an input script that reads a restart file. However, the coefficient information is not stored in the restart file, since it is tabulated in the potential files. Thus, angle_coeff commands do need to be specified in the restart input script.

20.42.4 Restrictions

This angle style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

20.42.5 Related commands

angle_coeff

Default: none

20.43 angle_style zero command

20.43.1 Syntax

```
angle_style zero *nocoeff*
```

20.43.2 Examples

```
angle_style zero
angle_style zero nocoeff
angle_coeff *
angle_coeff * 120.0
```

20.43.3 Description

Using an angle style of zero means angle forces and energies are not computed, but the geometry of angle triplets is still accessible to other commands.

As an example, the *compute angle/local* command can be used to compute the theta values for the list of triplets of angle atoms listed in the data file read by the *read_data* command. If no angle style is defined, this command cannot be used.

The optional *nocoeff* flag allows to read data files with AngleCoeff section for any angle style. Similarly, any *angle_coeff* commands will only be checked for the angle type number and the rest ignored.

Note that the *angle_coeff* command must be used for all angle types. If specified, there can be only one value, which is going to be used to assign an equilibrium angle, e.g. for use with *fix shake*.

20.43.4 Restrictions

none

20.43.5 Related commands

angle_style none

Default: none

CHAPTER

TWENTYONE

DIHEDRAL STYLES

21.1 dihedral_style charmm command

21.2 dihedral_style charmm/intel command

21.3 dihedral_style charmm/kk command

21.4 dihedral_style charmm/omp command

21.5 dihedral_style charmmfsw command

21.5.1 Syntax

```
dihedral_style style
```

- style = *charmm* or *charmmfsw*

21.5.2 Examples

```
dihedral_style charmm
dihedral_style charmmfsw
dihedral_coeff  1 0.2 1 180 1.0
dihedral_coeff  2 1.8 1   0 1.0
dihedral_coeff  1 3.1 2 180 0.5
```

21.5.3 Description

The *charmm* and *charmmfsw* dihedral styles use the potential

$$E = K[1 + \cos(n\phi - d)]$$

See *(MacKerell)* for a description of the CHARMM force field. This dihedral style can also be used for the AMBER force field (see comment on weighting factors below). See *(Cornell)* for a description of the AMBER force field.

Note: The newer *charmmfsw* style was released in March 2017. We recommend it be used instead of the older *charmm* style when running a simulation with the CHARMM force field, either with long-range Coulombics or a Coulombic cutoff, via the *pair_style lj/charmmfsw/coul/long* and *pair_style lj/charmmfsw/coul/charmmfsh* commands respectively. Otherwise the older *charmm* style is fine to use. See the discussion below and more details on the *pair_style charmm* doc page.

The following coefficients must be defined for each dihedral type via the *dihedral_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- n (integer >= 0)
- d (integer value of degrees)
- weighting factor (1.0, 0.5, or 0.0)

The weighting factor is required to correct for double counting pairwise non-bonded Lennard-Jones interactions in cyclic systems or when using the CHARMM dihedral style with non-CHARMM force fields. With the CHARMM dihedral style, interactions between the 1st and 4th atoms in a dihedral are skipped during the normal non-bonded force computation and instead evaluated as part of the dihedral using special epsilon and sigma values specified with the *pair_coeff* command of pair styles that contain "lj/charmm" (e.g. *pair_style lj/charmm/coul/long*) In 6-membered rings, the same 1-4 interaction would be computed twice (once for the clockwise 1-4 pair in dihedral 1-2-3-4 and once in the counterclockwise dihedral 1-6-5-4) and thus the weighting factor has to be 0.5 in this case. In 4-membered or 5-membered rings, the 1-4 dihedral also is counted as a 1-2 or 1-3 interaction when going around the ring in the opposite direction and thus the weighting factor is 0.0, as the 1-2 and 1-3 exclusions take precedence.

Note that this dihedral weighting factor is unrelated to the scaling factor specified by the *special bonds* command which applies to all 1-4 interactions in the system. For CHARMM force fields, the special_bonds 1-4 interaction scaling factor should be set to 0.0. Since the corresponding 1-4 non-bonded interactions are computed with the dihedral. This means that if any of the weighting factors defined as dihedral coefficients (4th coeff above) are non-zero, then you must use a pair style with "lj/charmm" and set the special_bonds 1-4 scaling factor to 0.0 (which is the default). Otherwise 1-4 non-bonded interactions in dihedrals will be computed twice.

For simulations using the CHARMM force field with a Coulombic cutoff, the difference between the *charmm* and *charmmfsw* styles is in the computation of the 1-4 non-bond interactions, though only if the distance between the two atoms is within the switching region of the pairwise potential defined by the corresponding CHARMM pair style, i.e. within the outer cutoff specified for the pair style. The *charmmfsw* style should only be used when using the corresponding *pair_style lj/charmmfsw/coul/charmmfsw* or *pair_style lj/charmmfsw/coul/long* commands. Use the *charmm* style with the older *pair_style* commands that have just "charmm" in their style name. See the discussion on the *CHARMM pair_style* doc page for details.

Note that for AMBER force fields, which use pair styles with "lj/cut", the special_bonds 1-4 scaling factor should be set to the AMBER defaults (1/2 and 5/6) and all the dihedral weighting factors (4th coeff above) must be set to 0.0. In this case, you can use any pair style you wish, since the dihedral does not need any Lennard-Jones parameter information and will not compute any 1-4 non-bonded interactions. Likewise the *charmm* or *charmmfsw* styles are identical in this case since no 1-4 non-bonded interactions are computed.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

21.5.4 Restrictions

When using run_style *respa*, these dihedral styles must be assigned to the same r-RESPA level as *pair* or *outer*.

When used in combination with CHARMM pair styles, the 1-4 *special_bonds* scaling factors must be set to 0.0. Otherwise non-bonded contributions for these 1-4 pairs will be computed multiple times.

These dihedral styles can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

21.5.5 Related commands

dihedral_coeff

Default: none

(Cornell) Cornell, Cieplak, Bayly, Gould, Merz, Ferguson, Spellmeyer, Fox, Caldwell, Kollman, JACS 117, 5179-5197 (1995).

(MacKerell) MacKerell, Bashford, Bellott, Dunbrack, Evanseck, Field, Fischer, Gao, Guo, Ha, et al, J Phys Chem B, 102, 3586 (1998).

21.6 dihedral_style class2 command

21.7 dihedral_style class2/omp command

21.8 dihedral_style class2/kk command

21.8.1 Syntax

```
dihedral_style class2
```

21.8.2 Examples

```
dihedral_style class2
dihedral_coeff 1 100 75 100 70 80 60
dihedral_coeff * mbt 3.5945 0.1704 -0.5490 1.5228
dihedral_coeff * ebt 0.3417 0.3264 -0.9036 0.1368 0.0 -0.8080 1.0119 1.1010
dihedral_coeff 2 at 0.0 -0.1850 -0.7963 -2.0220 0.0 -0.3991 110.2453 105.1270
dihedral_coeff * aat -13.5271 110.2453 105.1270
dihedral_coeff * bb13 0.0 1.0119 1.1010
```

21.8.3 Description

The *class2* dihedral style uses the potential

$$
\begin{aligned}
E =& E_d + E_{mbt} + E_{ebt} + E_{at} + E_{aat} + E_{bb13} \\
E_d =& \sum_{n=1}^{3} K_n[1 - \cos(n\phi - \phi_n)] \\
E_{mbt} =& (r_{jk} - r_2)[A_1 \cos(\phi) + A_2 \cos(2\phi) + A_3 \cos(3\phi)] \\
E_{ebt} =& (r_{ij} - r_1)[B_1 \cos(\phi) + B_2 \cos(2\phi) + B_3 \cos(3\phi)] + \\
& (r_{kl} - r_3)[C_1 \cos(\phi) + C_2 \cos(2\phi) + C_3 \cos(3\phi)] \\
E_{at} =& (\theta_{ijk} - \theta_1)[D_1 \cos(\phi) + D_2 \cos(2\phi) + D_3 \cos(3\phi)] + \\
& (\theta_{jkl} - \theta_2)[E_1 \cos(\phi) + E_2 \cos(2\phi) + E_3 \cos(3\phi)] \\
E_{aat} =& M(\theta_{ijk} - \theta_1)(\theta_{jkl} - \theta_2) \cos(\phi) \\
E_{bb13} =& N(r_{ij} - r_1)(r_{kl} - r_3)
\end{aligned}
$$

where E_d is the dihedral term, E_{mbt} is a middle-bond-torsion term, E_{ebt} is an end-bond-torsion term, E_{at} is an angle-torsion term, E_{aat} is an angle-angle-torsion term, and E_{bb13} is a bond-bond-13 term.

θ_1 and θ_2 are equilibrium angles and r_1, r_2, and r_3 are equilibrium bond lengths.

See *(Sun)* for a description of the COMPASS class2 force field.

Coefficients for the E_d, E_{mbt}, E_{ebt}, E_{at}, E_{aat}, and E_{bb13} formulas must be defined for each dihedral type via the *dihedral_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands.

These are the 6 coefficients for the E_d formula:

- K_1 (energy)
- ϕ_1 (degrees)
- K_2 (energy)
- ϕ_2 (degrees)
- K_3 (energy)
- phi_3 (degrees)

For the E_{mbt} formula, each line in a *dihedral_coeff* command in the input script lists 5 coefficients, the first of which is *mbt* to indicate they are MiddleBondTorsion coefficients. In a data file, these coefficients should be listed under a *MiddleBondTorsion Coeffs* heading and you must leave out the *mbt*, i.e. only list 4 coefficients after the dihedral type.

- *mbt*
- A_1 (energy/distance)
- A_2 (energy/distance)
- A_3 (energy/distance)
- r_2 (distance)

For the E_{ebt} formula, each line in a *dihedral_coeff* command in the input script lists 9 coefficients, the first of which is *ebt* to indicate they are EndBondTorsion coefficients. In a data file, these coefficients should be listed under a *EndBondTorsion Coeffs* heading and you must leave out the *ebt*, i.e. only list 8 coefficients after the dihedral type.

- *ebt*
- B_1 (energy/distance)

- B_2 (energy/distance)
- B_3 (energy/distance)
- C_1 (energy/distance)
- C_2 (energy/distance)
- C_3 (energy/distance)
- r_1 (distance)
- r_3 (distance)

For the E_{at} formula, each line in a *dihedral_coeff* command in the input script lists 9 coefficients, the first of which is *at* to indicate they are AngleTorsion coefficients. In a data file, these coefficients should be listed under a *AngleTorsion Coeffs* heading and you must leave out the *at*, i.e. only list 8 coefficients after the dihedral type.

- *at*
- D_1 (energy/radian)
- D_2 (energy/radian)
- D_3 (energy/radian)
- E_1 (energy/radian)
- E_2 (energy/radian)
- E_3 (energy/radian)
- θ_1 (degrees)
- θ_2 (degrees)

θ_1 and θ_2 are specified in degrees, but LAMMPS converts them to radians internally; hence the units of D and E are in energy/radian.

For the E_{aat} formula, each line in a *dihedral_coeff* command in the input script lists 4 coefficients, the first of which is *aat* to indicate they are AngleAngleTorsion coefficients. In a data file, these coefficients should be listed under a *AngleAngleTorsion Coeffs* heading and you must leave out the *aat*, i.e. only list 3 coefficients after the dihedral type.

- *aat*
- M (energy/radian^2)
- θ_1 (degrees)
- θ_2 (degrees)

θ_1 and θ_2 are specified in degrees, but LAMMPS converts them to radians internally; hence the units of M are in energy/radian^2.

For the E_{bb13} formula, each line in a *dihedral_coeff* command in the input script lists 4 coefficients, the first of which is *bb13* to indicate they are BondBond13 coefficients. In a data file, these coefficients should be listed under a *BondBond13 Coeffs* heading and you must leave out the *bb13*, i.e. only list 3 coefficients after the dihedral type.

- *bb13*
- N (energy/distance^2)
- r_1 (distance)
- r_3 (distance)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

21.8.4 Restrictions

This dihedral style can only be used if LAMMPS was built with the CLASS2 package. See the *Build package* doc page for more info.

21.8.5 Related commands

dihedral_coeff

Default: none

(Sun) Sun, J Phys Chem B 102, 7338-7364 (1998).

21.9 dihedral_style cosine/shift/exp command

21.10 dihedral_style cosine/shift/exp/omp command

21.10.1 Syntax

```
dihedral_style cosine/shift/exp
```

21.10.2 Examples

```
dihedral_style cosine/shift/exp
dihedral_coeff 1 10.0 45.0 2.0
```

21.10.3 Description

The *cosine/shift/exp* dihedral style uses the potential

$$E = -U_{min} \frac{e^{-aU(\theta,\theta_0)} - 1}{e^a - 1} \quad \text{with} \quad U(\theta,\theta_0) = -0.5\,(1 + \cos(\theta - \theta_0))$$

where U_{min}, θ, and a are defined for each dihedral type.

The potential is bounded between $[-U_{min} : 0]$ and the minimum is located at the angle θ_0. The a parameter can be both positive or negative and is used to control the spring constant at the equilibrium.

The spring constant is given by $k = ae^a \frac{U_{min}}{2(e^a-1)}$. For $a > 3$ and $\frac{k}{U_{min}} = \frac{a}{2}$ to better than 5% relative error. For negative values of the a parameter, the spring constant is essentially zero, and anharmonic terms takes over. The potential is furthermore well behaved in the limit $a \to 0$, where it has been implemented to linear order in a for $a < 0.001$.

The following coefficients must be defined for each dihedral type via the *dihedral_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- U_{min} (energy)
- θ (angle)
- a (real number)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

21.10.4 Restrictions

This dihedral style can only be used if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

21.10.5 Related commands

dihedral_coeff, *angle_style cosine/shift/exp*

Default: none

21.11 dihedral_style fourier command

21.12 dihedral_style fourier/intel command

21.13 dihedral_style fourier/omp command

21.13.1 Syntax

```
dihedral_style fourier
```

21.13.2 Examples

```
dihedral_style fourier
dihedral_coeff 1 3 -0.846200 3 0.0 7.578800 1 0 0.138000 2 -180.0
```

21.13.3 Description

The *fourier* dihedral style uses the potential:

$$E = \sum_{i=1,m} K_i[1.0 + \cos(n_i\phi - d_i)]$$

The following coefficients must be defined for each dihedral type via the *dihedral_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- m (integer >=1)
- K_1 (energy)
- n_1 (integer >= 0)
- d_1 (degrees)
- [...]
- K_m (energy)
- n_m (integer >= 0)
- d_m (degrees)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

21.13.4 Restrictions

This angle style can only be used if LAMMPS was built with the USER_MISC package. See the *Build package* doc page for more info.

21.13.5 Related commands

dihedral_coeff

Default: none

21.14 dihedral_style harmonic command

21.15 dihedral_style harmonic/intel command

21.16 dihedral_style harmonic/kk command

21.17 dihedral_style harmonic/omp command

21.17.1 Syntax

```
dihedral_style harmonic
```

21.17.2 Examples

```
dihedral_style harmonic
dihedral_coeff 1 80.0 1 2
```

21.17.3 Description

The *harmonic* dihedral style uses the potential

$$E = K[1 + d\cos(n\phi)]$$

The following coefficients must be defined for each dihedral type via the *dihedral_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- d (+1 or -1)
- n (integer >= 0)

Note: Here are important points to take note of when defining LAMMPS dihedral coefficients for the harmonic style, so that they are compatible with how harmonic dihedrals are defined by other force fields:

- The LAMMPS convention is that the trans position = 180 degrees, while in some force fields trans = 0 degrees.

- Some force fields reverse the sign convention on d.
- Some force fields let n be positive or negative which corresponds to $d = 1$ or $d = -1$ for the harmonic style.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

21.17.4 Restrictions

This dihedral style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

21.17.5 Related commands

dihedral_coeff

Default: none

21.18 dihedral_style helix command

21.19 dihedral_style helix/omp command

21.19.1 Syntax

```
dihedral_style helix
```

21.19.2 Examples

```
dihedral_style helix
dihedral_coeff 1 80.0 100.0 40.0
```

21.19.3 Description

The *helix* dihedral style uses the potential

$$E = A[1 - \cos(\theta)] + B[1 + \cos(3\theta)] + C[1 + \cos(\theta + \frac{\pi}{4})]$$

This coarse-grain dihedral potential is described in *(Guo)*. For dihedral angles in the helical region, the energy function is represented by a standard potential consisting of three minima, one corresponding to the trans (t) state and the other to gauche states (g+ and g-). The paper describes how the A, B and, C parameters are chosen so as to balance secondary (largely driven by local interactions) and tertiary structure (driven by long-range interactions).

The following coefficients must be defined for each dihedral type via the *dihedral_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- A (energy)
- B (energy)
- C (energy)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

21.19.4 Restrictions

This dihedral style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

21.19.5 Related commands

dihedral_coeff

Default: none

(Guo) Guo and Thirumalai, Journal of Molecular Biology, 263, 323-43 (1996).

21.20 dihedral_style hybrid command

21.20.1 Syntax

```
dihedral_style hybrid style1 style2 ...
```

- style1,style2 = list of one or more dihedral styles

21.20.2 Examples

```
dihedral_style hybrid harmonic helix
dihedral_coeff 1 harmonic 6.0 1 3
dihedral_coeff 2* helix 10 10 10
```

21.20.3 Description

The *hybrid* style enables the use of multiple dihedral styles in one simulation. An dihedral style is assigned to each dihedral type. For example, dihedrals in a polymer flow (of dihedral type 1) could be computed with a *harmonic* potential and dihedrals in the wall boundary (of dihedral type 2) could be computed with a *helix* potential. The assignment of dihedral type to style is made via the *dihedral_coeff* command or in the data file.

In the dihedral_coeff commands, the name of a dihedral style must be added after the dihedral type, with the remaining coefficients being those appropriate to that style. In the example above, the 2 dihedral_coeff commands set dihedrals of dihedral type 1 to be computed with a *harmonic* potential with coefficients 6.0, 1, 3 for K, d, n. All other dihedral types (2-N) are computed with a *helix* potential with coefficients 10, 10, 10 for A, B, C.

If dihedral coefficients are specified in the data file read via the *read_data* command, then the same rule applies. E.g. "harmonic" or "helix", must be added after the dihedral type, for each line in the "Dihedral Coeffs" section, e.g.

```
Dihedral Coeffs

1 harmonic 6.0 1 3
2 helix 10 10 10
...
```

If *class2* is one of the dihedral hybrid styles, the same rule holds for specifying additional AngleTorsion (and EndBondTorsion, etc) coefficients either via the input script or in the data file. I.e. *class2* must be added to each line after the dihedral type. For lines in the AngleTorsion (or EndBondTorsion, etc) section of the data file for dihedral types that are not *class2*, you must use an dihedral style of *skip* as a placeholder, e.g.

```
AngleTorsion Coeffs

1 skip
2 class2 1.0 1.0 1.0 3.0 3.0 3.0 30.0 50.0
...
```

Note that it is not necessary to use the dihedral style *skip* in the input script, since AngleTorsion (or EndBondTorsion, etc) coefficients need not be specified at all for dihedral types that are not *class2*.

A dihedral style of *none* with no additional coefficients can be used in place of a dihedral style, either in a input script dihedral_coeff command or in the data file, if you desire to turn off interactions for specific dihedral types.

21.20.4 Restrictions

This dihedral style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

Unlike other dihedral styles, the hybrid dihedral style does not store dihedral coefficient info for individual sub-styles in a *binary restart files*. Thus when restarting a simulation from a restart file, you need to re-specify dihedral_coeff commands.

21.20.5 Related commands

dihedral_coeff

Default: none

21.21 dihedral_style multi/harmonic command

21.22 dihedral_style multi/harmonic/omp command

21.22.1 Syntax

```
dihedral_style multi/harmonic
```

21.22.2 Examples

```
dihedral_style multi/harmonic
dihedral_coeff 1 20 20 20 20 20
```

21.22.3 Description

The *multi/harmonic* dihedral style uses the potential

$$E = \sum_{n=1,5} A_n \cos^{n-1}(\phi)$$

The following coefficients must be defined for each dihedral type via the *dihedral_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- A_1 (energy)
- A_2 (energy)
- A_3 (energy)
- A_4 (energy)
- A_5 (energy)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages*

doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

21.22.4 Restrictions

This dihedral style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

21.22.5 Related commands

dihedral_coeff

Default: none

21.23 dihedral_style nharmonic command

21.24 dihedral_style nharmonic/omp command

21.24.1 Syntax

```
dihedral_style nharmonic
```

21.24.2 Examples

```
dihedral_style nharmonic
dihedral_coeff * 3 10.0 20.0 30.0
```

21.24.3 Description

The *nharmonic* dihedral style uses the potential:

$$E = \sum_{n=1,n} A_n \cos^{n-1}(\phi)$$

The following coefficients must be defined for each dihedral type via the *dihedral_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- n (integer >=1)
- A_1 (energy)

- A_2 (energy)
- ...
- A_n (energy)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

21.24.4 Restrictions

This angle style can only be used if LAMMPS was built with the USER_MISC package. See the *Build package* doc page for more info.

21.24.5 Related commands

dihedral_coeff

Default: none

21.25 dihedral_style none command

21.25.1 Syntax

```
dihedral_style none
```

21.25.2 Examples

```
dihedral_style none
```

21.25.3 Description

Using a dihedral style of none means dihedral forces and energies are not computed, even if quadruplets of dihedral atoms were listed in the data file read by the *read_data* command.

See the *dihedral_style zero* command for a way to calculate dihedral statistics, but compute no dihedral interactions.

21.25.4 Restrictions

none

21.25.5 Related commands

dihedral_style zero

Default: none

21.26 dihedral_style opls command

21.27 dihedral_style opls/intel command

21.28 dihedral_style opls/kk command

21.29 dihedral_style opls/omp command

21.29.1 Syntax

```
dihedral_style opls
```

21.29.2 Examples

```
dihedral_style opls
dihedral_coeff 1 1.740 -0.157 0.279 0.00   # CT-CT-CT-CT
dihedral_coeff 2 0.000 0.000 0.366 0.000   # CT-CT-CT-HC
dihedral_coeff 3 0.000 0.000 0.318 0.000   # HC-CT-CT-HC
```

21.29.3 Description

The *opls* dihedral style uses the potential

$$E = \frac{1}{2}K_1[1+\cos(\phi)] + \frac{1}{2}K_2[1-\cos(2\phi)] + \frac{1}{2}K_3[1+\cos(3\phi)] + \frac{1}{2}K_4[1-\cos(4\phi)]$$

Note that the usual 1/2 factor is not included in the K values.

This dihedral potential is used in the OPLS force field and is described in *(Watkins)*.

The following coefficients must be defined for each dihedral type via the *dihedral_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K_1 (energy)
- K_2 (energy)
- K_3 (energy)
- K_4 (energy)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

21.29.4 Restrictions

This dihedral style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

21.29.5 Related commands

dihedral_coeff

Default: none

(Watkins) Watkins and Jorgensen, J Phys Chem A, 105, 4118-4125 (2001).

21.30 dihedral_style quadratic command

21.31 dihedral_style quadratic/omp command

21.31.1 Syntax

```
dihedral_style quadratic
```

21.31.2 Examples

```
dihedral_style quadratic
dihedral_coeff 100.0 80.0
```

21.31.3 Description

The *quadratic* dihedral style uses the potential:

$$E = K(\phi - \phi_0)^2$$

This dihedral potential can be used to keep a dihedral in a predefined value (cis=zero, right-hand convention is used).

The following coefficients must be defined for each dihedral type via the *dihedral_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy/radian^2)
- ϕ_0 (degrees)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

21.31.4 Restrictions

This angle style can only be used if LAMMPS was built with the USER_MISC package. See the *Build package* doc page for more info.

21.31.5 Related commands

dihedral_coeff

Default: none

21.32 dihedral_style spherical command

21.32.1 Syntax

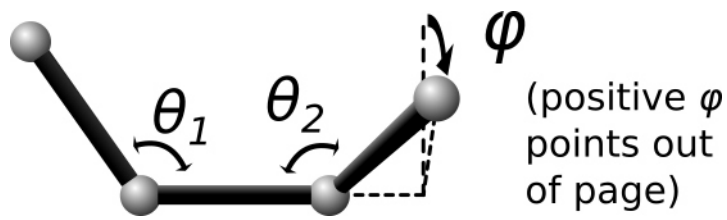
```
dihedral_style spherical
```

21.32.2 Examples

```
dihedral_coeff 1 1  286.1  1 124  1    1 90.0 0    1 90.0 0
dihedral_coeff 1 3  69.3   1 93.9 1    1 90   0    1 90   0  &
                    49.1   0 0.00 0    1 74.4 1    0 0.00 0  &
                    25.2   0 0.00 0    0 0.00 0    1 48.1 1
```

21.32.3 Description

The *spherical* dihedral style uses the potential:



$$E(\phi,\theta_1,\theta_2) = \sum_{i=1}^{N} C_i\,\Phi_i(\phi)\,\Theta_{1i}(\theta_1)\,\Theta_{2i}(\theta_2)$$
$$\Phi_i(\phi) = u_i - \cos((\phi - a_i)K_i)$$
$$\Theta_{1i}(\theta_1) = v_i - \cos((\theta_1 - b_i)L_i)$$
$$\Theta_{2i}(\theta_2) = w_i - \cos((\theta_2 - c_i)M_i)$$

For this dihedral style, the energy can be any function that combines the 4-body dihedral-angle (ϕ) and the two 3-body bond-angles (θ_1, θ_2). For this reason, there is usually no need to define 3-body "angle" forces separately for the atoms participating in these interactions. It is probably more efficient to incorporate 3-body angle forces into the dihedral interaction even if it requires adding additional terms to the expansion (as was done in the second example). A careful choice of parameters can prevent singularities that occur with traditional force-fields whenever theta1 or theta2 approach 0 or 180 degrees.

The last example above corresponds to an interaction with a single energy minima located near $\phi = 93.9$, $\theta_1 = 74.4$, $\theta_2 = 48.1$ degrees, and it remains numerically stable at all angles (ϕ, θ_1, θ_2). In this example, the coefficients 49.1, and 25.2 can be physically interpreted as the harmonic spring constants for theta1 and theta2 around their minima. The coefficient 69.3 is the harmonic spring constant for phi after division by sin(74.4)*sin(48.1) (the minima positions for theta1 and theta2).

The following coefficients must be defined for each dihedral type via the *dihedral_coeff* command as in the example above, or in the Dihedral Coeffs section of a data file read by the *read_data* command:

- n (integer >= 1)
- C_1 (energy)
- K_1 (typically an integer)
- a_1 (degrees)

- u_1 (typically 0.0 or 1.0)
- L_1 (typically an integer)
- b_1 (degrees, typically 0.0 or 90.0)
- v_1 (typically 0.0 or 1.0)
- M_1 (typically an integer)
- c_1 (degrees, typically 0.0 or 90.0)
- w_1 (typically 0.0 or 1.0)
- [...]
- C_n (energy)
- K_n (typically an integer)
- a_n (degrees)
- u_n (typically 0.0 or 1.0)
- L_n (typically an integer)
- b_n (degrees, typically 0.0 or 90.0)
- v_n (typically 0.0 or 1.0)
- M_n (typically an integer)
- c_n (degrees, typically 0.0 or 90.0)
- w_n (typically 0.0 or 1.0)

21.32.4 Restrictions

This dihedral style can only be used if LAMMPS was built with the USER_MISC package. See the *Build package* doc page for more info.

21.32.5 Related commands

dihedral_coeff

Default: none

21.33 dihedral_style table command

21.34 dihedral_style table/omp command

21.34.1 Syntax

```
dihedral_style table style Ntable
```

- style = *linear* or *spline* = method of interpolation
- Ntable = size of the internal lookup table

21.34.2 Examples

```
dihedral_style table spline 400
dihedral_style table linear 1000
dihedral_coeff 1 file.table DIH_TABLE1
dihedral_coeff 2 file.table DIH_TABLE2
```

21.34.3 Description

The *table* dihedral style creates interpolation tables of length *Ntable* from dihedral potential and derivative values listed in a file(s) as a function of the dihedral angle "phi". The files are read by the *dihedral_coeff* command.

The interpolation tables are created by fitting cubic splines to the file values and interpolating energy and derivative values at each of *Ntable* dihedral angles. During a simulation, these tables are used to interpolate energy and force values on individual atoms as needed. The interpolation is done in one of 2 styles: *linear* or *spline*.

For the *linear* style, the dihedral angle (phi) is used to find 2 surrounding table values from which an energy or its derivative is computed by linear interpolation.

For the *spline* style, cubic spline coefficients are computed and stored at each of the *Ntable* evenly-spaced values in the interpolated table. For a given dihedral angle (phi), the appropriate coefficients are chosen from this list, and a cubic polynomial is used to compute the energy and the derivative at this angle.

The following coefficients must be defined for each dihedral type via the *dihedral_coeff* command as in the example above.

- filename
- keyword

The filename specifies a file containing tabulated energy and derivative values. The keyword specifies a section of the file. The format of this file is described below.

The format of a tabulated file is as follows (without the parenthesized comments). It can begin with one or more comment or blank lines.

```
# Table of the potential and its negative derivative

DIH_TABLE1                    (keyword is the first text on line)
N 30 DEGREES                  (N, NOF, DEGREES, RADIANS, CHECKU/F)
                              (blank line)
1 -168.0 -1.40351172223 0.0423346818422
2 -156.0 -1.70447981034 0.00811786522531
3 -144.0 -1.62956100432 -0.0184129719987
...
30 180.0 -0.707106781187 0.0719306095245

# Example 2: table of the potential. Forces omitted

DIH_TABLE2
N 30 NOF CHECKU testU.dat CHECKF testF.dat

1 -168.0 -1.40351172223
2 -156.0 -1.70447981034
3 -144.0 -1.62956100432
...
30 180.0 -0.707106781187
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the *dihedral_coeff* command. The next line lists (in any order) one or more parameters for the table. Each parameter is a keyword followed by one or more numeric values.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is the angle value, the 3rd value is the energy (in energy units), and the 4th is -dE/d(phi) also in energy units). The 3rd term is the energy of the 4-atom configuration for the specified angle. The 4th term (when present) is the negative derivative of the energy with respect to the angle (in degrees, or radians depending on whether the user selected DEGREES or RADIANS). Thus the units of the last term are still energy, not force. The dihedral angle values must increase from one line to the next.

Dihedral table splines are cyclic. There is no discontinuity at 180 degrees (or at any other angle). Although in the examples above, the angles range from -180 to 180 degrees, in general, the first angle in the list can have any value (positive, zero, or negative). However the *range* of angles represented in the table must be *strictly* less than 360 degrees (2pi radians) to avoid angle overlap. (You may not supply entries in the table for both 180 and -180, for example.) If the user's table covers only a narrow range of dihedral angles, strange numerical behavior can occur in the large remaining gap.

Parameters:

The parameter "N" is required and its value is the number of table entries that follow. Note that this may be different than the N specified in the *dihedral_style table* command. Let *Ntable* is the number of table entries requested dihedral_style command, and let *Nfile* be the parameter following "N" in the tabulated file ("30" in the sparse example above). What LAMMPS does is a preliminary interpolation by creating splines using the *Nfile* tabulated values as nodal points. It uses these to interpolate as needed to generate energy and derivative values at *Ntable* different points (which are evenly spaced over a 360 degree range, even if the angles in the file are not). The resulting tables of length *Ntable* are then used as described above, when computing energy and force for individual dihedral angles and their atoms. This means that if you want the interpolation tables of length *Ntable* to match exactly what is in the tabulated file (with effectively nopreliminary interpolation), you should set *Ntable* = *Nfile*. To insure the nodal points in the user's file are aligned with the interpolated table entries, the angles in the table should be integer multiples of 360/*Ntable* degrees, or 2*PI/*Ntable* radians (depending on your choice of angle units).

The optional "NOF" keyword allows the user to omit the forces (negative energy derivatives) from the table file (normally located in the 4th column). In their place, forces will be calculated automatically by differentiating the potential energy function indicated by the 3rd column of the table (using either linear or spline interpolation).

The optional "DEGREES" keyword allows the user to specify angles in degrees instead of radians (default).

The optional "RADIANS" keyword allows the user to specify angles in radians instead of degrees. (Note: This changes the way the forces are scaled in the 4th column of the data file.)

The optional "CHECKU" keyword is followed by a filename. This allows the user to save all of the *Ntable* different entries in the interpolated energy table to a file to make sure that the interpolated function agrees with the user's expectations. (Note: You can temporarily increase the *Ntable* parameter to a high value for this purpose. "*Ntable*" is explained above.)

The optional "CHECKF" keyword is analogous to the "CHECKU" keyword. It is followed by a filename, and it allows the user to check the interpolated force table. This option is available even if the user selected the "NOF" option.

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

Restart info:

This dihedral style writes the settings for the "dihedral_style table" command to *binary restart files*, so a dihedral_style command does not need to specified in an input script that reads a restart file. However, the coefficient information is not stored in the restart file, since it is tabulated in the potential files. Thus, dihedral_coeff commands do need to be specified in the restart input script.

21.34.4 Restrictions

This dihedral style can only be used if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

21.34.5 Related commands

dihedral_coeff

Default: none

21.35 dihedral_style table/cut command

21.35.1 Syntax

```
dihedral_style table/cut style Ntable
```

- style = *linear* or *spline* = method of interpolation
- Ntable = size of the internal lookup table

21.35.2 Examples

```
dihedral_style table/cut spline 400
dihedral_style table/cut linear 1000
dihedral_coeff 1 aat 1.0 177 180 file.table DIH_TABLE1
dihedral_coeff 2 aat 0.5 170 180 file.table DIH_TABLE2
```

21.35.3 Description

The *table/cut* dihedral style creates interpolation tables of length *Ntable* from dihedral potential and derivative values listed in a file(s) as a function of the dihedral angle "phi". In addition, an analytic cutoff that is quadratic in the bond-angle (theta) is applied in order to regularize the dihedral interaction. The dihedral table files are read by the *dihedral_coeff* command.

The interpolation tables are created by fitting cubic splines to the file values and interpolating energy and derivative values at each of *Ntable* dihedral angles. During a simulation, these tables are used to interpolate energy and force values on individual atoms as needed. The interpolation is done in one of 2 styles: *linear* or *spline*.

For the *linear* style, the dihedral angle (phi) is used to find 2 surrounding table values from which an energy or its derivative is computed by linear interpolation.

For the *spline* style, cubic spline coefficients are computed and stored at each of the *Ntable* evenly-spaced values in the interpolated table. For a given dihedral angle (phi), the appropriate coefficients are chosen from this list, and a cubic polynomial is used to compute the energy and the derivative at this angle.

The following coefficients must be defined for each dihedral type via the *dihedral_coeff* command as in the example above.

- style (aat)
- cutoff prefactor
- cutoff angle1
- cutoff angle2
- filename
- keyword

The cutoff dihedral style uses a tabulated dihedral interaction with a cutoff function:

$$f(\theta) = K \qquad \theta < \theta_1$$
$$f(\theta) = K\left(1 - \frac{(\theta-\theta_1)^2}{(\theta_2-\theta_1)^2}\right) \qquad \theta_1 < \theta < \theta_2$$

The cutoff specifies an prefactor to the cutoff function. While this value would ordinarily equal 1 there may be situations where the value should change.

The cutoff θ_1 specifies the angle (in degrees) below which the dihedral interaction is unmodified, i.e. the cutoff function is 1.

The cutoff function is applied between θ_1 and θ_2, which is the angle at which the cutoff function drops to zero. The value of zero effectively "turns off" the dihedral interaction.

The filename specifies a file containing tabulated energy and derivative values. The keyword specifies a section of the file. The format of this file is described below.

The format of a tabulated file is as follows (without the parenthesized comments). It can begin with one or more comment or blank lines.

```
# Table of the potential and its negative derivative

DIH_TABLE1                    (keyword is the first text on line)
N 30 DEGREES                  (N, NOF, DEGREES, RADIANS, CHECKU/F)
                              (blank line)
1 -168.0 -1.40351172223 0.0423346818422
```

(continues on next page)

(continued from previous page)

```
2 -156.0 -1.70447981034 0.00811786522531
3 -144.0 -1.62956100432 -0.0184129719987
...
30 180.0 -0.707106781187 0.0719306095245

# Example 2: table of the potential. Forces omitted

DIH_TABLE2
N 30 NOF CHECKU testU.dat CHECKF testF.dat

1 -168.0 -1.40351172223
2 -156.0 -1.70447981034
3 -144.0 -1.62956100432
...
30 180.0 -0.707106781187
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the *dihedral_coeff* command. The next line lists (in any order) one or more parameters for the table. Each parameter is a keyword followed by one or more numeric values.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is the angle value, the 3rd value is the energy (in energy units), and the 4th is -dE/d(phi) also in energy units). The 3rd term is the energy of the 4-atom configuration for the specified angle. The 4th term (when present) is the negative derivative of the energy with respect to the angle (in degrees, or radians depending on whether the user selected DEGREES or RADIANS). Thus the units of the last term are still energy, not force. The dihedral angle values must increase from one line to the next.

Dihedral table splines are cyclic. There is no discontinuity at 180 degrees (or at any other angle). Although in the examples above, the angles range from -180 to 180 degrees, in general, the first angle in the list can have any value (positive, zero, or negative). However the *range* of angles represented in the table must be *strictly* less than 360 degrees (2pi radians) to avoid angle overlap. (You may not supply entries in the table for both 180 and -180, for example.) If the user's table covers only a narrow range of dihedral angles, strange numerical behavior can occur in the large remaining gap.

Parameters:

The parameter "N" is required and its value is the number of table entries that follow. Note that this may be different than the N specified in the *dihedral_style table* command. Let *Ntable* is the number of table entries requested dihedral_style command, and let *Nfile* be the parameter following "N" in the tabulated file ("30" in the sparse example above). What LAMMPS does is a preliminary interpolation by creating splines using the *Nfile* tabulated values as nodal points. It uses these to interpolate as needed to generate energy and derivative values at *Ntable* different points (which are evenly spaced over a 360 degree range, even if the angles in the file are not). The resulting tables of length *Ntable* are then used as described above, when computing energy and force for individual dihedral angles and their atoms. This means that if you want the interpolation tables of length *Ntable* to match exactly what is in the tabulated file (with effectively nopreliminary interpolation), you should set *Ntable* = *Nfile*. To insure the nodal points in the user's file are aligned with the interpolated table entries, the angles in the table should be integer multiples of 360/*Ntable* degrees, or 2*PI/*Ntable* radians (depending on your choice of angle units).

The optional "NOF" keyword allows the user to omit the forces (negative energy derivatives) from the table file (normally located in the 4th column). In their place, forces will be calculated automatically by differentiating the potential energy function indicated by the 3rd column of the table (using either linear or spline interpolation).

The optional "DEGREES" keyword allows the user to specify angles in degrees instead of radians (default).

The optional "RADIANS" keyword allows the user to specify angles in radians instead of degrees. (Note: This

changes the way the forces are scaled in the 4th column of the data file.)

The optional "CHECKU" keyword is followed by a filename. This allows the user to save all of the *Ntable* different entries in the interpolated energy table to a file to make sure that the interpolated function agrees with the user's expectations. (Note: You can temporarily increase the *Ntable* parameter to a high value for this purpose. "*Ntable*" is explained above.)

The optional "CHECKF" keyword is analogous to the "CHECKU" keyword. It is followed by a filename, and it allows the user to check the interpolated force table. This option is available even if the user selected the "NOF" option.

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

Restart info:

This dihedral style writes the settings for the "dihedral_style table/cut" command to *binary restart files*, so a dihedral_style command does not need to specified in an input script that reads a restart file. However, the coefficient information is not stored in the restart file, since it is tabulated in the potential files. Thus, dihedral_coeff commands do need to be specified in the restart input script.

21.35.4 Restrictions

This dihedral style can only be used if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

21.35.5 Related commands

dihedral_coeff, *dihedral_style table*

Default: none

(Salerno) Salerno, Bernstein, J Chem Theory Comput, –, —- (2018).

21.36 dihedral_style zero command

21.36.1 Syntax

```
dihedral_style zero [nocoeff]
```

21.36.2 Examples

```
dihedral_style zero
dihedral_style zero nocoeff
dihedral_coeff *
```

21.36.3 Description

Using a dihedral style of zero means dihedral forces and energies are not computed, but the geometry of dihedral quadruplets is still accessible to other commands.

As an example, the *compute dihedral/local* command can be used to compute the theta values for the list of quadruplets of dihedral atoms listed in the data file read by the *read_data* command. If no dihedral style is defined, this command cannot be used.

The optional *nocoeff* flag allows to read data files with a DihedralCoeff section for any dihedral style. Similarly, any dihedral_coeff commands will only be checked for the dihedral type number and the rest ignored.

Note that the *dihedral_coeff* command must be used for all dihedral types, though no additional values are specified.

21.36.4 Restrictions

none

Related commands: none

dihedral_style none

Default: none

CHAPTER

TWENTYTWO

IMPROPER STYLES

22.1 improper_style class2 command

22.2 improper_style class2/omp command

22.3 improper_style class2/kk command

22.3.1 Syntax

```
improper_style class2
```

22.3.2 Examples

```
improper_style class2
improper_coeff 1 100.0 0
improper_coeff * aa 0.0 0.0 0.0 115.06 130.01 115.06
```

22.3.3 Description

The *class2* improper style uses the potential

$$
\begin{aligned}
E =& E_i + E_{aa} \\
E_i =& K[\frac{\chi_{ijkl} + \chi_{kjli} + \chi_{ljik}}{3} - \chi_0]^2 \\
E_{aa} =& M_1(\theta_{ijk} - \theta_1)(\theta_{kjl} - \theta_3) + \\
& M_2(\theta_{ijk} - \theta_1)(\theta_{ijl} - \theta_2) + \\
& M_3(\theta_{ijl} - \theta_2)(\theta_{kjl} - \theta_3)
\end{aligned}
$$

where E_i is the improper term and E_{aa} is an angle-angle term. The 3 χ terms in E_i are an average over 3 out-of-plane angles.

The 4 atoms in an improper quadruplet (listed in the data file read by the *read_data* command) are ordered I,J,K,L. χ_{ijkl} refers to the angle between the plane of I,J,K and the plane of J,K,L, and the bond JK lies in both planes. Similarly for χ_{kjli} and χ_{ljik}. Note that atom J appears in the common bonds (JI, JK, JL) of all 3 X terms. Thus J (the 2nd atom in the quadruplet) is the atom of symmetry in the 3 χ angles.

The subscripts on the various θs refer to different combinations of 3 atoms (I,J,K,L) used to form a particular angle. E.g. θ_{ijl} is the angle formed by atoms I,J,L with J in the middle. θ_1, θ_2, θ_3 are the equilibrium positions of those angles. Again, atom J (the 2nd atom in the quadruplet) is the atom of symmetry in the theta angles, since it is always the center atom.

Since atom J is the atom of symmetry, normally the bonds J-I, J-K, J-L would exist for an improper to be defined between the 4 atoms, but this is not required.

See *(Sun)* for a description of the COMPASS class2 force field.

Coefficients for the E_i and E_{aa} formulas must be defined for each improper type via the *improper_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands.

These are the 2 coefficients for the E_i formula:

- K (energy/radian^2)
- χ_0 (degrees)

χ_0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of K are in energy/radian^2.

For the E_{aa} formula, each line in a *improper_coeff* command in the input script lists 7 coefficients, the first of which is *aa* to indicate they are AngleAngle coefficients. In a data file, these coefficients should be listed under a *AngleAngle Coeffs* heading and you must leave out the *aa*, i.e. only list 6 coefficients after the improper type.

- *aa*
- M_1 (energy/distance)
- M_2 (energy/distance)
- M_3 (energy/distance)
- θ_1 (degrees)
- θ_2 (degrees)
- θ_3 (degrees)

The theta values are specified in degrees, but LAMMPS converts them to radians internally; hence the units of M are in energy/radian^2.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

22.3.4 Restrictions

This improper style can only be used if LAMMPS was built with the CLASS2 package. See the *Build package* doc page for more info.

22.3.5 Related commands

improper_coeff

Default: none

(Sun) Sun, J Phys Chem B 102, 7338-7364 (1998).

22.4 improper_style cossq command

22.5 improper_style cossq/omp command

22.5.1 Syntax

```
improper_style cossq
```

22.5.2 Examples

```
improper_style cossq
improper_coeff 1 4.0 0.0
```

22.5.3 Description

The *cossq* improper style uses the potential

$$E = \frac{1}{2} K \cos^2 (\chi - \chi_0)$$

where χ is the improper angle, χ_0 is its equilibrium value, and K is a prefactor.

If the 4 atoms in an improper quadruplet (listed in the data file read by the *read_data* command) are ordered I,J,K,L then χ is the angle between the plane of I,J,K and the plane of J,K,L. Alternatively, you can think of atoms J,K,L as being in a plane, and atom I above the plane, and χ as a measure of how far out-of-plane I is with respect to the other 3 atoms.

Note that defining 4 atoms to interact in this way, does not mean that bonds necessarily exist between I-J, J-K, or K-L, as they would in a linear dihedral. Normally, the bonds I-J, I-K, I-L would exist for an improper to be defined between the 4 atoms.

The following coefficients must be defined for each improper type via the *improper_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- χ_0 (degrees)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

22.5.4 Restrictions

This improper style can only be used if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

22.5.5 Related commands

improper_coeff

Default: none

22.6 improper_style cvff command

22.7 improper_style cvff/intel command

22.8 improper_style cvff/omp command

22.8.1 Syntax

```
improper_style cvff
```

22.8.2 Examples

```
improper_style cvff
improper_coeff 1 80.0 -1 4
```

22.8.3 Description

The *cvff* improper style uses the potential

$$E = K[1 + d\cos(n\phi)]$$

where phi is the improper dihedral angle.

If the 4 atoms in an improper quadruplet (listed in the data file read by the *read_data* command) are ordered I,J,K,L then the improper dihedral angle is between the plane of I,J,K and the plane of J,K,L. Note that because this is effectively a dihedral angle, the formula for this improper style is the same as for *dihedral_style harmonic*.

Note that defining 4 atoms to interact in this way, does not mean that bonds necessarily exist between I-J, J-K, or K-L, as they would in a linear dihedral. Normally, the bonds I-J, I-K, I-L would exist for an improper to be defined between the 4 atoms.

The following coefficients must be defined for each improper type via the *improper_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- d (+1 or -1)
- n (0,1,2,3,4,6)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

22.8.4 Restrictions

This improper style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

22.8.5 Related commands

improper_coeff

Default: none

22.9 improper_style distance command

22.9.1 Syntax

```
improper_style distance
```

22.9.2 Examples

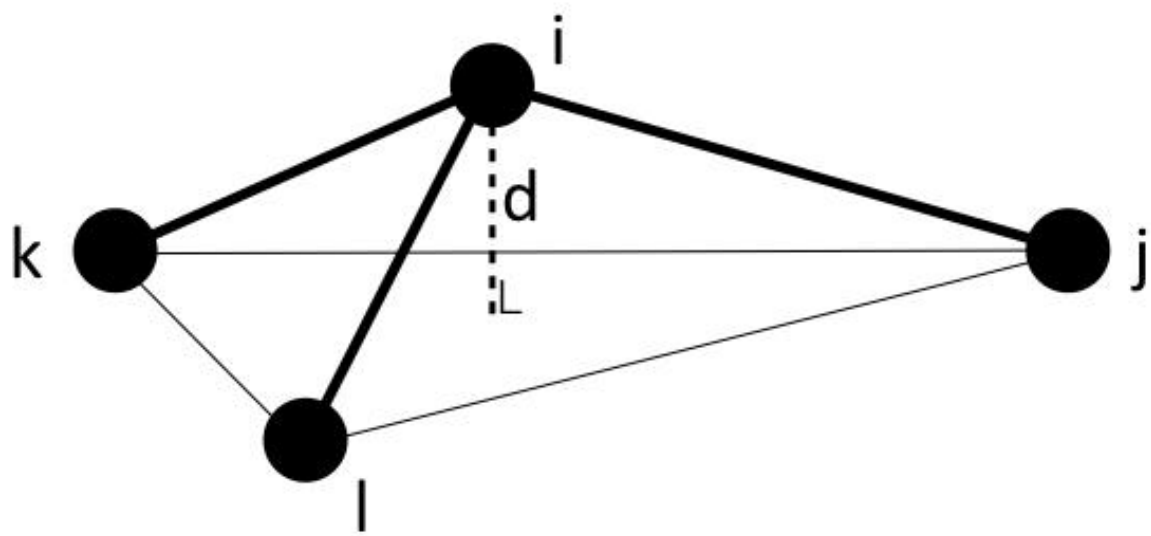
```
improper_style distance
improper_coeff 1 80.0 100.0
```

22.9.3 Description

The *distance* improper style uses the potential

$$E = K_2 d^2 + K_4 d^4$$

where d is the distance between the central atom and the plane formed by the other three atoms. If the 4 atoms in an improper quadruplet (listed in the data file read by the *read_data* command) are ordered I,J,K,L then the I-atom is assumed to be the central atom.



Note that defining 4 atoms to interact in this way, does not mean that bonds necessarily exist between I-J, J-K, or K-L, as they would in a linear dihedral. Normally, the bonds I-J, I-K, I-L would exist for an improper to be defined between the 4 atoms.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K_2 (energy/distance^2)
- K_4 (energy/distance^4)

22.9.4 Restrictions

This improper style can only be used if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

22.9.5 Related commands

improper_coeff

Default: none

22.10 improper_style distharm command

22.10.1 Syntax

```
improper_style distharm
```

22.10.2 Examples

```
improper_style distharm
improper_coeff 1 25.0 0.5
```

22.10.3 Description

The *distharm* improper style uses the potential

$$E = K(d - d_0)^2$$

where d is the oriented distance between the central atom and the plane formed by the other three atoms. If the 4 atoms in an improper quadruplet (listed in the data file read by the *read_data* command) are ordered I,J,K,L then the L-atom is assumed to be the central atom. Note that this is different from the convention used in the improper_style distance. The distance d is oriented and can take on negative values. This may lead to unwanted behavior if d_0 is not equal to zero.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy/distance^2)
- d_0 (distance)

22.10.4 Restrictions

This improper style can only be used if LAMMPS was built with the USER-YAFF package. See the *Build package* doc page for more info.

22.10.5 Related commands

improper_coeff

Default: none

22.11 improper_style fourier command

22.12 improper_style fourier/omp command

22.12.1 Syntax

```
improper_style fourier
```

22.12.2 Examples

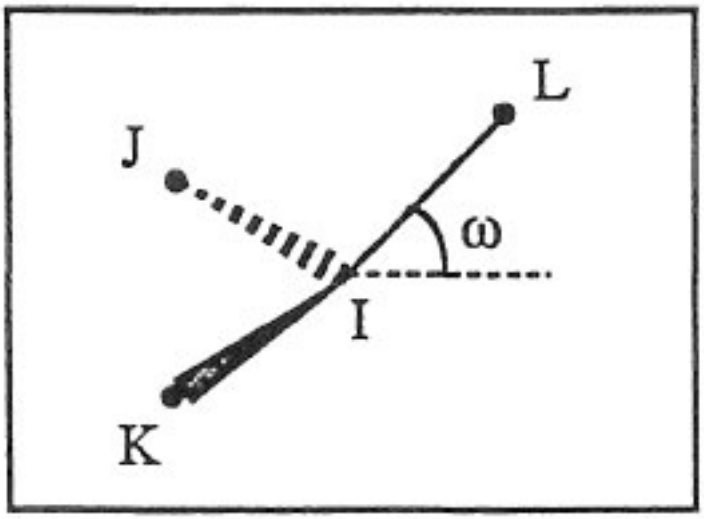
```
improper_style fourier
improper_coeff 1 100.0 0.0 1.0 0.5 1
```

22.12.3 Description

The *fourier* improper style uses the following potential:

$$E = K[C_0 + C_1 \cos(\omega) + C_2 \cos(2\omega)]$$

where K is the force constant, C0, C1, C2 are dimensionless coefficients, and omega is the angle between the IL axis and the IJK plane:



If all parameter (see below) is not zero, the all the three possible angles will taken in account.

The following coefficients must be defined for each improper type via the *improper_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- C_0 (unitless)
- C_1 (unitless)
- C_2 (unitless)
- all (0 or 1, optional)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

22.12.4 Restrictions

This angle style can only be used if LAMMPS was built with the USER_MISC package. See the *Build package* doc page for more info.

22.12.5 Related commands

improper_coeff

Default: none

22.13 improper_style harmonic command

22.14 improper_style harmonic/intel command

22.15 improper_style harmonic/kk command

22.16 improper_style harmonic/omp command

22.16.1 Syntax

```
improper_style harmonic
```

22.16.2 Examples

```
improper_style harmonic
improper_coeff 1 100.0 0
```

22.16.3 Description

The *harmonic* improper style uses the potential

$$E = K(\chi - \chi_0)^2$$

where χ is the improper angle, χ_0 is its equilibrium value, and K is a prefactor. Note that the usual 1/2 factor is included in K.

If the 4 atoms in an improper quadruplet (listed in the data file read by the *read_data* command) are ordered I,J,K,L then χ is the angle between the plane of I,J,K and the plane of J,K,L. Alternatively, you can think of atoms J,K,L as being in a plane, and atom I above the plane, and χ as a measure of how far out-of-plane I is with respect to the other 3 atoms.

Note that defining 4 atoms to interact in this way, does not mean that bonds necessarily exist between I-J, J-K, or K-L, as they would in a linear dihedral. Normally, the bonds I-J, I-K, I-L would exist for an improper to be defined between the 4 atoms.

The following coefficients must be defined for each improper type via the *improper_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy/radian^2)
- χ_0 (degrees)

χ_0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of K are in energy/radian^2.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

22.16.4 Restrictions

This improper style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

22.16.5 Related commands

improper_coeff

Default: none

22.17 improper_style hybrid command

22.17.1 Syntax

```
improper_style hybrid style1 style2 ...
```

- style1,style2 = list of one or more improper styles

22.17.2 Examples

```
improper_style hybrid harmonic helix
improper_coeff 1 harmonic 120.0 30
improper_coeff 2 cvff 20.0 -1 2
```

22.17.3 Description

The *hybrid* style enables the use of multiple improper styles in one simulation. An improper style is assigned to each improper type. For example, impropers in a polymer flow (of improper type 1) could be computed with a *harmonic* potential and impropers in the wall boundary (of improper type 2) could be computed with a *cvff* potential. The assignment of improper type to style is made via the *improper_coeff* command or in the data file.

In the improper_coeff command, the first coefficient sets the improper style and the remaining coefficients are those appropriate to that style. In the example above, the 2 improper_coeff commands would set impropers of improper type 1 to be computed with a *harmonic* potential with coefficients 120.0, 30 for K, χ_0. Improper type 2 would be computed with a *cvff* potential with coefficients 20.0, -1, 2 for K, d, and n, respectively.

If the improper *class2* potential is one of the hybrid styles, it requires additional AngleAngle coefficients be specified in the data file. These lines must also have an additional "class2" argument added after the improper type. For improper types which are assigned to other hybrid styles, use the style name (e.g. "harmonic") appropriate to that style. The AngleAngle coeffs for that improper type will then be ignored.

An improper style of *none* can be specified as the 2nd argument to the improper_coeff command, if you desire to turn off certain improper types.

22.17.4 Restrictions

This improper style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

Unlike other improper styles, the hybrid improper style does not store improper coefficient info for individual sub-styles in a *binary restart files*. Thus when restarting a simulation from a restart file, you need to re-specify improper_coeff commands.

22.17.5 Related commands

improper_coeff

Default: none

22.18 improper_style inversion/harmonic command

22.18.1 Syntax

```
improper_style inversion/harmonic
```

22.18.2 Examples

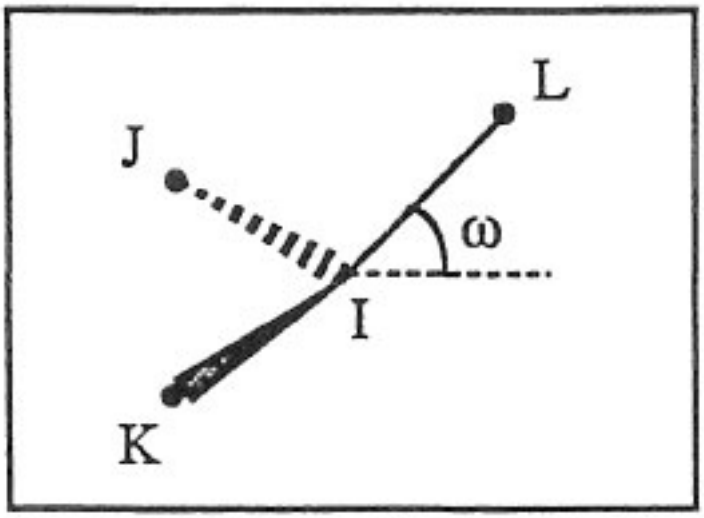
```
improper_style inversion/harmonic
improper_coeff 1 18.776340 0.000000
```

22.18.3 Description

The *inversion/harmonic* improper style follows the Wilson-Decius out-of-plane angle definition and uses an harmonic potential:

$$E = K\left(\omega - \omega_0\right)^2$$

where K is the force constant and ω is the angle evaluated for all three axis-plane combinations centered around the atom I. For the IL axis and the IJK plane ω looks as follows:



Note that the *inversion/harmonic* angle term evaluation differs to the *improper_umbrella* due to the cyclic evaluation of all possible angles ω.

The following coefficients must be defined for each improper type via the *improper_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- ω_0 (degrees)

If $\omega_0 = 0$ the potential term has a single minimum for the planar structure. Otherwise it has two minima at +/- ω_0, with a barrier in between.

22.18.4 Restrictions

This improper style can only be used if LAMMPS was built with the USER-MOFFF package. See the *Build package* doc page for more info.

22.18.5 Related commands

improper_coeff

Default: none

22.19 improper_style none command

22.19.1 Syntax

```
improper_style none
```

22.19.2 Examples

```
improper_style none
```

22.19.3 Description

Using an improper style of none means improper forces and energies are not computed, even if quadruplets of improper atoms were listed in the data file read by the *read_data* command.

See the *improper_style zero* command for a way to calculate improper statistics, but compute no improper interactions.

22.19.4 Restrictions

none

22.19.5 Related commands

improper_style zero

Default: none

22.20 improper_style ring command

22.21 improper_style ring/omp command

22.21.1 Syntax

```
improper_style ring
```

22.21.2 Examples

```
improper_style ring
improper_coeff 1 8000 70.5
```

22.21.3 Description

The *ring* improper style uses the potential

$$
\begin{aligned}
E =& \frac{1}{6} K \left(\Delta_{ijl} + \Delta_{ijk} + \Delta_{kjl}\right)^6 \\
\Delta_{ijl} =& \cos\theta_{ijl} - \cos\theta_0 \\
\Delta_{ijk} =& \cos\theta_{ijk} - \cos\theta_0 \\
\Delta_{kjl} =& \cos\theta_{kjl} - \cos\theta_0
\end{aligned}
$$

where K is a prefactor, θ is the angle formed by the atoms specified by (i,j,k,l) indices and θ_0 its equilibrium value.

If the 4 atoms in an improper quadruplet (listed in the data file read by the *read_data* command) are ordered i,j,k,l then theta_*ijl* is the angle between atoms i,j and l, theta_*ijk* is the angle between atoms i,j and k, theta_*kjl* is the angle between atoms j,k, and l.

The "ring" improper style implements the improper potential introduced by Destree et al., in Equation (9) of *(Destree)*. This potential does not affect small amplitude vibrations but is used in an ad-hoc way to prevent the onset of accidentally large amplitude fluctuations leading to the occurrence of a planar conformation of the three bonds i-j, j-k and j-l, an intermediate conformation toward the chiral inversion of a methine carbon. In the "Impropers" section of data file four atoms: i, j, k and l are specified with i,j and l lying on the backbone of the chain and k specifying the chirality of j.

The following coefficients must be defined for each improper type via the *improper_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- θ_0 (degrees)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

22.21.4 Restrictions

This improper style can only be used if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

22.21.5 Related commands

improper_coeff

(Destree) M. Destree, F. Laupretre, A. Lyulin, and J.-P. Ryckaert, J Chem Phys, 112, 9632 (2000).

22.22 improper_style sqdistharm command

22.22.1 Syntax

```
improper_style sqdistharm
```

22.22.2 Examples

```
improper_style sqdistharm
improper_coeff 1 50.0 0.1
```

22.22.3 Description

The *sqdistharm* improper style uses the potential

$$E = K(d^2 - {d_0}^2)^2$$

where d is the distance between the central atom and the plane formed by the other three atoms. If the 4 atoms in an improper quadruplet (listed in the data file read by the *read_data* command) are ordered I,J,K,L then the L-atom is assumed to be the central atom. Note that this is different from the convention used in the improper_style distance.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy/distance^4)
- ${d_0}^2$ (distance^2)

Note that ${d_0}^2$ (in units distance^2) has be provided and not d_0.

22.22.4 Restrictions

This improper style can only be used if LAMMPS was built with the USER-MISC package. See the *Build package* doc page for more info.

22.22.5 Related commands

improper_coeff

Default: none

22.23 improper_style umbrella command

22.24 improper_style umbrella/omp command

22.24.1 Syntax

```
improper_style umbrella
```

22.24.2 Examples

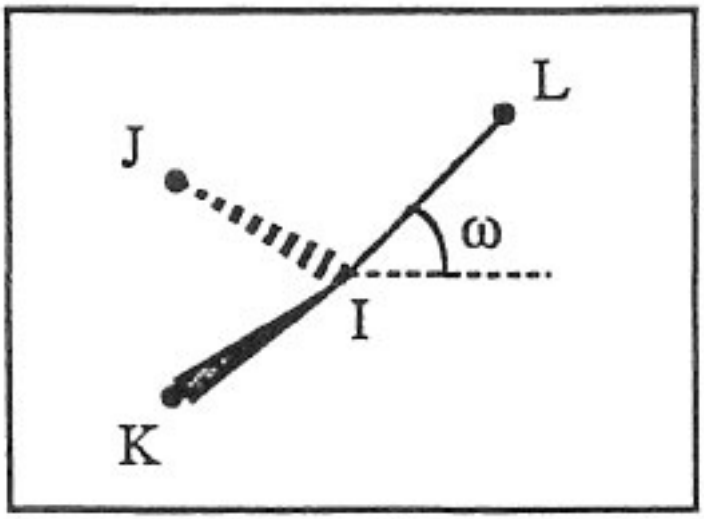
```
improper_style umbrella
improper_coeff 1 100.0 180.0
```

22.24.3 Description

The *umbrella* improper style uses the following potential, which is commonly referred to as a classic inversion and used in the *DREIDING* force field:

$$E = \frac{1}{2} K \left(\frac{1}{\sin \omega_0} \right)^2 (\cos \omega - \cos \omega_0)^2 \qquad \omega_0 \neq 0^o$$
$$E = K\,(1 - cos\omega) \qquad \omega_0 = 0^o$$

where K is the force constant and ω is the angle between the IL axis and the IJK plane:



If $\omega_0 = 0$ the potential term has a minimum for the planar structure. Otherwise it has two minima at $\omega + / - \omega_0$, with a barrier in between.

See *(Mayo)* for a description of the DREIDING force field.

The following coefficients must be defined for each improper type via the *improper_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- ω_0 (degrees)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Speed packages* doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Speed packages* doc page for more instructions on how to use the accelerated styles effectively.

22.24.4 Restrictions

This improper style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

22.24.5 Related commands

improper_coeff

Default: none

(Mayo) Mayo, Olfason, Goddard III, J Phys Chem, 94, 8897-8909 (1990),

22.25 improper_style zero command

22.25.1 Syntax

```
improper_style zero [nocoeff]
```

22.25.2 Examples

```
improper_style zero
improper_style zero nocoeff
improper_coeff *
```

22.25.3 Description

Using an improper style of zero means improper forces and energies are not computed, but the geometry of improper quadruplets is still accessible to other commands.

As an example, the *compute improper/local* command can be used to compute the chi values for the list of quadruplets of improper atoms listed in the data file read by the *read_data* command. If no improper style is defined, this command cannot be used.

The optional *nocoeff* flag allows to read data files with a ImproperCoeff section for any improper style. Similarly, any improper_coeff commands will only be checked for the improper type number and the rest ignored.

Note that the *improper_coeff* command must be used for all improper types, though no additional values are specified.

22.25.4 Restrictions

none

Related commands: none

improper_style none

Default: none

CHAPTER

TWENTYTHREE

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