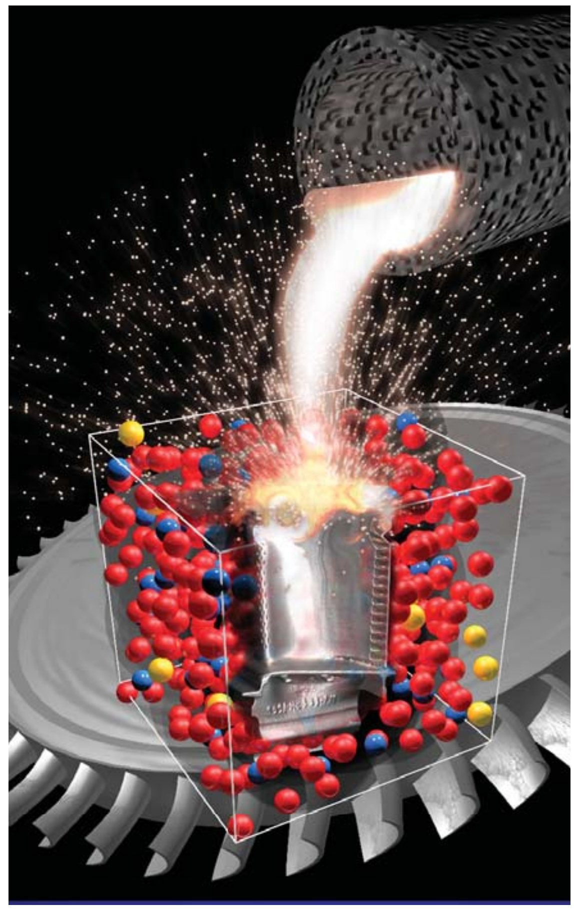
Molecular Dynamics Simulate the Molten State of Super Alloys for Tomorrow's Aircraft

Project Purpose: *Enable advances in aerospace propulsion by predicting fundamental material parameters controlling the processing of high performance turbine airfoils.*

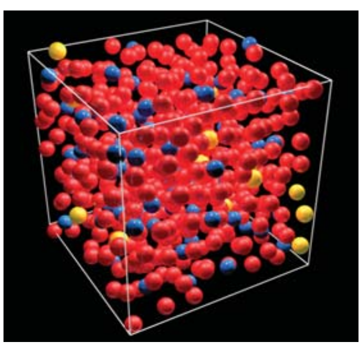
Some Like it Hot:

Physics tells us that the efficiency of turbine engines is controlled by the temperature difference between the incoming air and that of the air-fuel mixture ignited in the combustion chamber. Realizing this, engineers have driven the turbine gas flow temperatures above the melting temperatures of the airfoils used to drive these systems. Turbine airfoils are highly engineered components made from specialized materials, called Ni-based Superalloys, that are capable of carrying huge loads at very high temperatures. Often airfoil designs call for active cooling, where complex cooling channels and holes are used to blow cool air inside and around the working blade. In order to produce these complex geometries and requisite properties, airfoils are made using advanced casting methods. As materials and designs evolve to increase performance, making these components often produce casting (freckle) defects that severely degrade material performance.



Graphic representation of computational assistance for studying hot molten alloys forming turbine engine blades for high performance jet aircraft.

Using HPC resources, Drs. C. Woodward and J. Lill are predicting fundamental materials parameters (i.e. density, diffusion, and viscosity) that influence the convective flow that produces these defects. These numerical methods offer a predictive tool for molten superalloy properties that are extremely difficult to measure experimentally. This information informs modern process models and will enable advances in component and materials design leading to improved turbine engine efficiencies.



Snapshot from a quantum mechanical simulation of a liquid alloy of Nickel, Aluminum, and Tungsten at 1711 degrees Kelvin, or about 2620 degrees Fahrenheit. The simulation has 500 atoms total: 410 Nickel (red), 78 Aluminum (blue), and 12 Tungsten (yellow)

IMPACTS:

- *Decreases the cost of casting expensive turbine blades*
- *Increases the dependability of critical engine parts*
- *Extends the performance and efficiencies of turbine jet engines*
- *Reduces development time for new super alloys*

Christopher Woodward, Materials and Manufacturing Directorate, AFRL Wright-Patterson AFB, OH, investigator of this Challenge project, which currently utilizes the AFRL DSRC HPC Systems Hawk and Raptor. This project has a total allocation of 2,600,000 hours on Hawk and 758,000 hours on Raptor. In addition, this project has performed many successful runs using HPC codes VASP, and Plane-Wave Self Consistent Field.