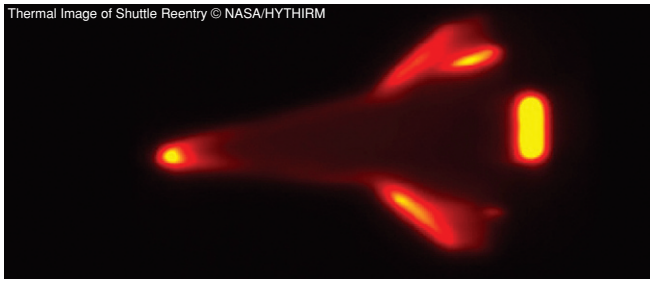
materials design

MedeA Thermal Conductivity

The MedeA Thermal Conductivity module harnesses today's computing power and computational methods to predict thermal conductivity for bulk materials as well as nanostructured systems, thus providing unprecedented capabilities for scientists and engineers. The Thermal Conductivity module takes advantage of the high parallel performance of LAMMPS and combines Materials Design's expertise in forcefields, simulations, and software engineering. With MedeA Thermal Conductivity, you can explore pure bulk phases, the effects of interfaces (Kapitza resistance), impurities, isotopic purity, and nanostructure on the thermal conductivity of your systems.

Key Benefits of MedeA Thermal Conductivity:

- *Handles all computational details, letting you focus on the science*
- *Allows you to easily set up complex calculations with powerful flowchart interface, and recall them later to either rerun or to edit before running again*
- *Provides an automatic analysis including fitting of results*
- *Validates data based on graphs, fitting errors and all intermediate results through convenient web interface*
- *Works with the JobServer and TaskServer to run your calculations on the appropriate hardware, centralizing the results*
- *Integrates with MedeA Forcefield for advanced forcefield handling and assignment*


Thermal Image of Shuttle Reentry © NASA/HYTHIRM

Required MedeA modules:

- *Core MedeA environment*
- *MedeA Forcefield*
- *MedeA LAMMPS*
- *JobServer and TaskServers*

Computational characteristics:

- *Uses the LAMMPS forcefield engine for high performance on any computer from a scalar workstation to a massively parallel cluster*
- *Provides the lattice component of the thermal conductivity. For insulators, and semiconductors at moderate temperatures, this is essentially all of the thermal conductivity.*
- *Reverse non-equilibrium methods (RNEMD), applicable to all systems*
  - *Requires elongated cells in the direction of conduction*
  - *Higher conductivities, which arise from longer phonon mean free path lengths, require correspondingly longer cells*
  - *The effect of the cell cross section must be examined*
  - *Transfer rate of heat must be optimized, requiring some user intervention*
- *Equilibrium molecular dynamics (EMD) Green-Kubo method for systems with no atomic charges*
  - *Requires moderate system sizes*
  - *Length of simulation depends on the thermal conductivity: higher conductivities require longer simulation times*
  - *Reasonable approximation for systems with small atomic charges, such as hydrocarbons, many semiconductor alloys, etc.*
  - *More automated than RNEMD methods*
- *Compatible with any forcefield handled by MedeA Forcefield*

Visit our website ***www.materialsdesign.com*** *or contact your local Materials Design office for further information.*

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