MedeA Thermal Conductivity

Quantify Heat Transport Characteristics of Materials

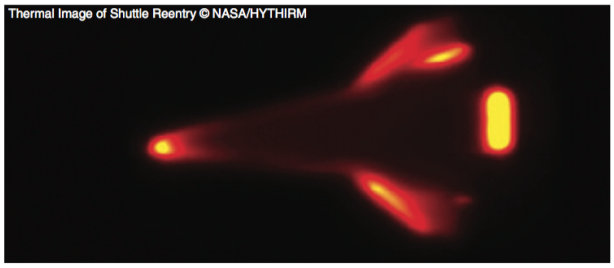
At-a-Glance

The *MedeA* ®[1] *Thermal Conductivity* module harnesses today's computing power and computational methods to predict thermal conductivity for bulk solid and liquid materials, and nanostructured systems. This powerful module employs both equilibrium and non-equilibrium classical simulation methods to provide information essential for the optimal design of advanced products and component materials.

MedeA Thermal Conductivity takes advantage of the parallel performance of LAMMPS, and it combines Materials Design's expertise in forcefields, simulations, and software engineering. With MedeA Thermal Conductivity, explore pure bulk phases, and examine the effects of interfaces (i.e. Thermal Boundary, or 'Kapitza', resistance), impurities, isotopic purity, and nanostructure on the thermal conductivity of your materials systems.

Key Benefits

- Handles all computational details, letting you focus on the science
- Allows easy set up of complex calculations using the powerful flowchart interface, as well as recall, to modify conditions or specify a different model before running again
- Provides automatic analysis, including fitting of results with uncertainty estimation
- Validates data based on graphs, including fitting errors and all intermediate results, through the convenient web interface
- Works with JobServer and TaskServer to run your calculations on the appropriate hardware, centralizing the results
- Integrates with MedeA Forcefields for advanced forcefield handling and assignment of a wide variety of organic, inorganic, and metallic materials



'The equilibrium molecular dynamics method within MedeA's thermal conductivity module makes it easy to perform routine property estimates on homogeneous non-metallic solids and liquids, while the complementary non-equilibrium method is particularly useful for making quantitative assessments of the effect of interfaces on heat transfer in complex multiphase materials.'

Computational Characteristics

- Uses the LAMMPS simulation engine for maximum performance on any computer, whether it be a scalar workstation or a massively parallel cluster
- Provides the lattice component of the thermal conductivity for ordered systems. For insulators and semiconductors at moderate temperatures, this is essentially all of the thermal conductivity
- Equilibrium molecular dynamics (EMD) Green-Kubo method:
  - Requires moderate system sizes
  - Requires variable simulation times: duration of simulation depends on the thermal conductivity, for example: higher

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conductivities require longer simulation times
  - More automated than RNEMD methods - simply build and equilibrate the system, and run
- Reverse non-equilibrium methods (RNEMD) method:
  - Requires elongated cells in the direction of conduction
  - Extrapolation vs. cell length for crystalline materials
  - Probes higher conductivities, which arise from longer phonon mean free path lengths, and require correspondingly longer cells
  - Optimizes imposed heat transfer rate, requiring some user intervention
  - The effect of the cell cross section may sometimes need to be examined
- Compatible with any of the forcefields handled by MedeA Forcefield

Required Modules

- *MedeA Environment*
- *MedeA Forcefield*
- *MedeA LAMMPS*
- *MedeA JobServer and TaskServer*

Find Out More

Learn more about how *MedeA Thermal Conductivity* has been used to study heat transfer and thermal boundary (Kapitza) resistance in advanced electronics devices in the review MedeA: Atomistic simulations for designing and testing materials for micro/nano electronics systems.

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