materials design

MedeA LAMMPS

The MedeA LAMMPS module provides flexible calculation setup and analysis capabilities to unlock the power of LAMMPS. LAMMPS is one of the leading forcefield-based molecular dynamics codes in the world today. Developed at Sandia National Laboratories by Steve Plimpton and his team, LAMMPS focuses on the highly efficient execution of forcefield-based simulations designed to exploit large-scale parallel computer architectures.

Key Benefits of MedeA LAMMPS:

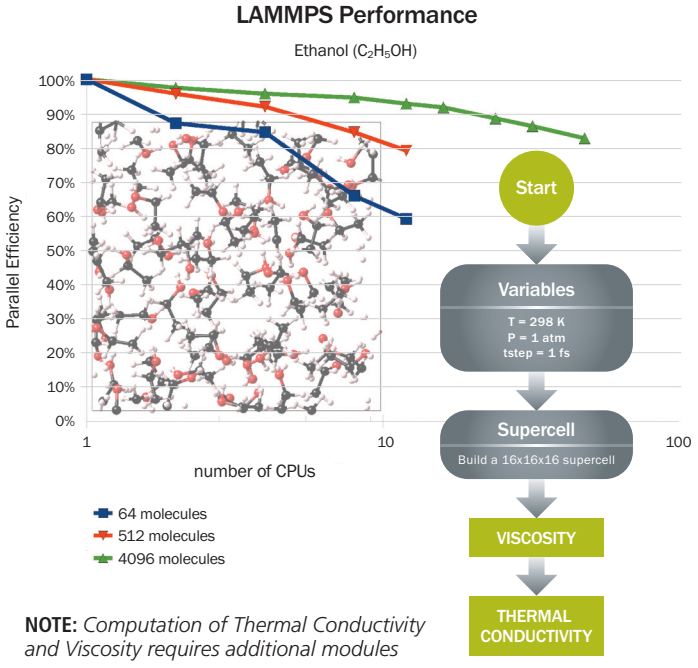
- *Automates the details of getting a molecule or solid and its associated forcefield parameters into the format needed by LAMMPS gaining time and reducing chances of errors*
- *Powerful flowchart interface lets you easily set up complex calculations by connecting stages*
  - *A stage can be a computation, e.g. energy minimization, NVT and NPT dynamics, as well as an operation such as setting the density to that computed by a previous stage, or building a larger simulation box*
  - *Any number of stages can be chained together to perform a detailed, reproducible calculation. For example, you may wish initially to equilibrate the system, then adjust the pressure, and finally run a long simulation to extract properties*
  - *Flowcharts from any previous calculation can be edited and run again, even on different molecules*
  - *Capture best practices, and share validated computational strategies with colleagues*
- *Automatic analysis of the results, including graphs, fitting to appropriate forms, and statistical analysis*
- *Quick verification of all final and intermediate results through a convenient web interface*
- *Works with the MedeA JobServer and TaskServer to run your calculations on the appropriate, possibly distributed hardware while keeping the results well organized with the JobServer*
- *Integrated with MedeA Forcefield for advanced forcefield handling and assignment*

Required MedeA modules:

- *Core MedeA environment*
- *MedeA Forcefield*
- *JobServer and TaskServer*

Computational Characteristics:

- *Uses the LAMMPS forcefield engine for high performance on any computer from a scalar workstation to a massively parallel cluster*
- *Provides access to the core capabilities of LAMMPS: minimization and molecular dynamics*
- *Built in analysis of standard properties, such as density, volume, and energies*
- *Visualization of trajectories*
- *"Custom" stages where you can directly add LAMMPS commands to handle applications not covered in the interface*
- *Compatible with any forcefield handled by MedeA Forcefield, including your own forcefield as long as it is in the format handled by MedeA Forcefield*



NOTE: *Computation of Thermal Conductivity and Viscosity requires additional modules*

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

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