materials design

MedeA Viscosity: Reliable Properties from Simulations

Take advantage of the power of the LAMMPS forcefield engine, combined with our expertise in both forcefields and simulations, to calculate the viscosity of pure fluids or of mixtures at a wide range of temperatures and pressures. MedeA Viscosity is based on the MedeA LAMMPS module. It adds a specialized, automated, and validated capability for the calculation of the viscosity through either equilibrium molecular dynamics (EMD) methods or nonequilibrium molecular dynamics (NMED) approaches.

Key Benefits of MedeA Viscosity:

- *Handles the complexity of calculating the viscosity in LAMMPS, letting you focus on the science*
- *Allows you to easily set up complex calculations with MedeA's powerful flowchart interface, and recall them later to either rerun or to edit before running again. See MedeA LAMMPS for more details*
- *Provides automatic analysis of the viscosity with graphs and fitting of the results, the numerical value of the viscosity, and statistical error bars*
- *Validates calculations through graphs and all intermediate results through a 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*

Computational characteristics:

- *Uses the LAMMPS forcefield engine for high performance on any computer from a scalar workstation to a massively parallel cluster*
- *Scales consistently with system size and the size of the computational cluster: if you double the system but run on twice as many cpu's, the computational time is unchanged*
- *Equilibrium molecular dynamics (EMD) Green-Kubo method for all systems*
  - *Requires moderate boxes of fluid*
  - *Length of simulation required depends on viscosity: the higher the viscosity the longer the calculation needed*
  - *Typical fluids with viscosities ~1 cP require 5-20 ns simulation time*
- *Reverse nonequilibrium methods (RNEMD) for all systems*
  - *Requires elongated and sometimes large boxes of fluids*
  - *Calculation time may be less than EMD methods; however, the optimal box cross section and momentum transfer rate must be determined, requiring more user intervention*
- *Compatible with any forcefield handled by MedeA Forcefield*

Required MedeA modules:

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

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

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