MedeA LAMMPS

A Powerful Gateway to a Powerful Simulation Program

At-a-Glance

MedeA ®[1] *LAMMPS* provides flexible calculation setup and analysis capabilities to unlock the power of LAMMPS.

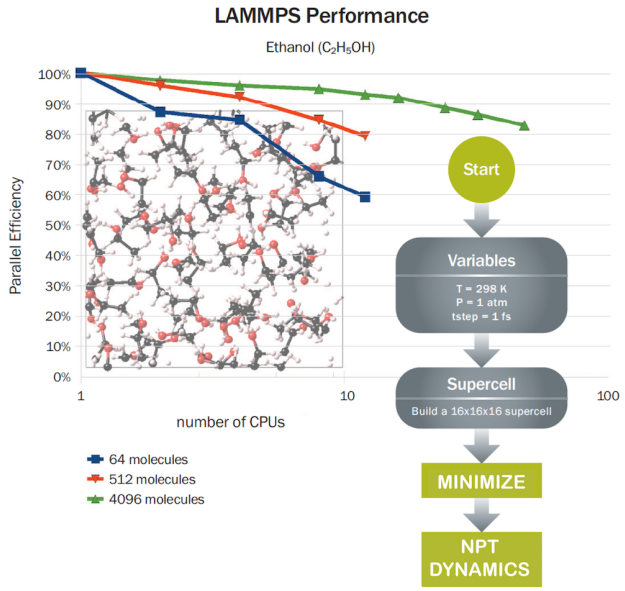
LAMMPS[2] is one of the world's leading forcefield-based molecular dynamics codes. Developed at Sandia National Laboratories by Steve Plimpton and fellow researchers, it enables highly efficient execution of forcefield based simulations in order to exploit large scale parallel and GPU-enabled computer architectures.

Key Benefits

- Saves time and avoids mistakes by preparing complex input structure files in seconds rather than hours or days
- Generates commands needed to run simulations automatically, without having to learn the language and syntax in detail
- Identifies all required forcefield terms and assigns appropriate parameters according to the chosen forcefield
- Analyzes key property output, and performs statistical analysis to determine averages and precision (error bars)

Specifications

- Uses the LAMMPS forcefield engine for high performance on any computer, whether it be a scalar workstation or a massively parallel cluster
- Runs on Windows (Server 2008/2012/2016, 7/8/10) and Linux (CentOS, Red Hat, Ubuntu, Debian, SUSE)
- Supports 64-bit CPU architectures and computers with GPU cards[3]
- *MedeA LAMMPS* calculations runs on an unlimited number of server computers or compute cores



'Setting up LAMMPS calculations on complex models using the flowchart interface is a significant productivity enhancer, and accumulating results in tables with the option to add occasional custom commands is very powerful indeed'

Key Features

- *MedeA LAMMPS* automates the details of properly formatting molecules, fluids, or solids into the required LAMMPS coordinate, connectivity, forcefield parameter, and command-line formats
- Provides access to the core capabilities of LAMMPS:
  - Minimization

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

[2] S.J. Plimpton, "Fast Parallel Algorithms for Short–Range Molecular Dynamics", *J. Comp. Phys.* **117**, 1 (1995) DOI

[3] Please contact Materials Design for information on the latest GPU cards tested for use with *MedeA-LAMMPS*

  - Molecular Dynamics simulations within the *NVE*, *NVT*, and *NPT* ensembles
  - Energy and Energy Derivative (force) calculation
- Works with the *MedeA JobServer and TaskServer* to run your calculations on the appropriate, possibly distributed, hardware, while keeping the results well organized within the JobServer
- Quick verification of all final and intermediate results through the convenient MedeA JobServer web browser interface
- Full integration with *MedeA Forcefield* for advanced forcefield handling and assignment
- Any custom forcefield which is provided in the appropriate *MedeA Forcefield* format is compatible
- Powerful *MedeA Flowcharts* enable you to set up complex calculations with ease by graphically connecting stages
- Flowcharts from any previous *MedeA-LAMMPS* calculation can be re-used, edited, shared with colleagues, and rerun, even on different systems and compute servers
- Provides options for expert LAMMPS users to add any LAMMPS commands to existing protocols, or to prepare completely customized simulations

Properties

- After each calculation, *MedeA LAMMPS* automatically determines the block averages and fluctuations of:
  - Temperature
  - Pressure
  - Density
  - Cell parameters
  - Total energy and all components (potential, kinetic, Coulomb, and van der Waals)
  - Stress tensor elements
- Visualization of trajectories of MD simulations and structure optimizations

Required Modules

- *MedeA Environment*

Recommended Modules

- *MedeA HT-Launchpad*
- *MedeA Amorphous Materials Builder*

Supported Modules

- *MedeA CED*
- *MedeA Diffusion*
- *MedeA Surface Tension*
- *MedeA Thermal Conductivity*
- *MedeA Viscosity*
- *MedeA Mechanical Properties (MT)*
- *MedeA COMB3*
- *MedeA EAM*

Tightly Integrated Modules

- *MedeA Forcefield Optimizer*
- *MedeA HT-Descriptor*
- *MedeA Phonon*
- *MedeA UNCLE*

Find Out More

Learn more about how *MedeA LAMMPS* can be used to study a broad range of inorganic, metallic, semiconductor, and organic materials by viewing the following webinar:

Harness the Power of LAMMPS Molecular Dynamics Code with MedeA

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