Teaching with LAMMPS

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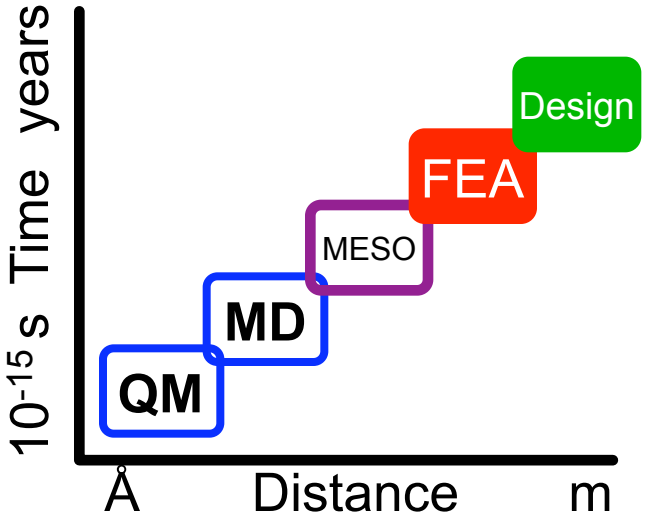
LAMMPS Workshop

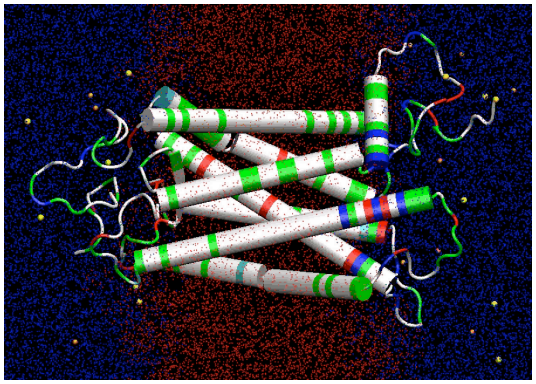
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

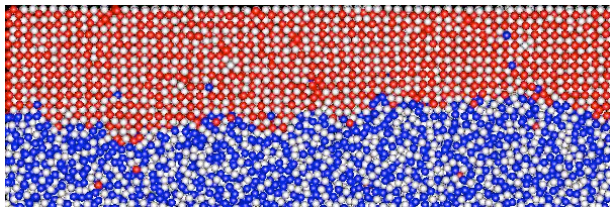
LAMMPS scope and examples

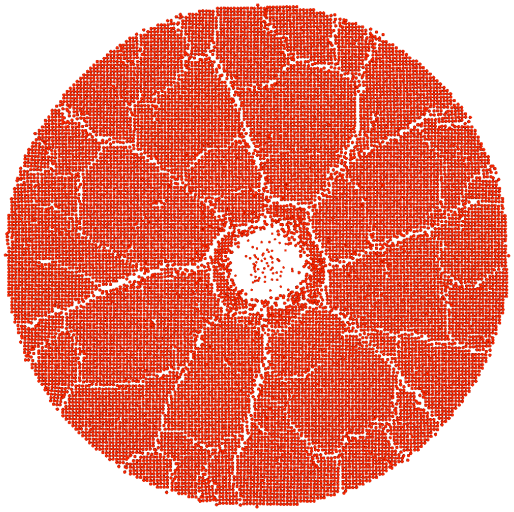
Large-scale **A**tomic/**M**olecular **M**assively **P**arallel **S**imulator

- LAMMPS is open-source (GNU Public License)
- ~50,000 LAMMPS downloads since Sept 2004.
- Three primary communities are supported by force fields, boundary conditions and diagnostics:
  - Biomolecules and polymers (soft materials)
  - Solids materials science
  - Mesoscale to continuum









Agenda

- Discrete Element Modeling Course at Texas
- TMS/MatDL and education for ICME-related codes
- Survey of current efforts
- Discussion

Discrete Element Modeling Course at Texas

- Course Description/Goals
  - Graduate-level semester course with modular lectures on the fundamentals of MD & MC
  - LAMMPS (www.lammps.sandia.gov) will be the platform for demos & student homework
  - This course should equip students to use and develop/modify LAMMPS for research
- Strategy and Format
  - One lecture per week by a Sandia staff member or UT faculty over 15-week semester
  - Major group project using LAMMPS to investigate a problem in materials science or engineering

    Application areas: MD algorithms, colloid suspension dynamics, granular flow, predictive properties of systems at equilibrium (e.g. phase change, microstructure), etc.
  - Class size in the 15-25 students range – all masters level
- Short-term schedule & Long-term vision
  - First course offering will be Spring 2011.
  - At Texas, the course will eventually be taught by senior grad student, with faculty advising.
  - The course will eventually be offered to Sandia staff, post-docs and interns, as well.

Proposed syllabus (draft)

Week 1: Overview of MD & MC. Approachable problems, length/time scales, scaling arguments

MOLECULAR DYNAMICS

Week 2: LAMMPS fundamentals/overview, tutorials, syntax and hands-on.

Week 3: Model system initialization tools. Visualization tools. Group project discussion

Week 4: Numerical methods and algorithms for solving discrete Newton's equations of motion.

Time integration, Ensemble averaging, Boundary conditions, Thermostat and barostat methods

Week 5: Methods for solvent systems

Brownian dynamics, Fully-explicit solvent, Dissipative particle dynamics, Stochastic rotation dynamics

Week 6: Property concepts and calculations

Diffusion, Viscosity, Surface tension, Phase separation, Melt temperature

PAIRWISE AND MULTIBODY INTERACTIONS

Week 7-8: Particle potentials through applications.

Colloidal and nanoparticle suspensions, solid mechanics, granular systems

MONTE CARLO

Week 9: Sampling Techniques

Week 10: Phase Equilibration

Week 11: Property Calculations – e.g. equations of state

Week 12: Demonstration problems. e.g., Aspherical particles. Other advanced topics.

PROJECT PRESENTATIONS

Week 13-15: Project completion. Group presentations.

TMS/MatDL and ICME-related codes

- ICME concept and TMS investment
  - Integrated Computational Materials Engineering
  - Hierarchy of material codes with common I/O
  - TMS funds projects which promote ICME goals through education

- Materials Digital Library (MatDL) Program
  - Funded through NSF and TMS
  - Neutral, central location for materials science codes
  - Store, manage and vet educational resources for participating codes
  - Pre-compiled linux boot CDs with standard distributions

LAMMPS participated in a roundtable with faculty at the TMS annual meeting focused on integrating material science codes into appropriate undergraduate courses

Survey results – user experience

1. Have you used LAMMPS in an educational setting?

   No, not a single respondent had used LAMMPS to teach.

2. Are you contemplating using LAMMPS for education in the future?

   Yes, 8 of 10 of responses. 3 had concrete near-term plans.

3. Have you developed classroom demonstrations, examples, assignments or student projects which utilize LAMMPS?

   No one had done any resource development.

Survey results – user experience (cont)

- Are there specific issues which might complicate using LAMMPS in your teaching?

  Access to clusters, Students unable to compile code, Students expect GUI. However, most say no obstacles.

- Would you be interested in additional resources for teaching with LAMMPS?

  9 of 10 responses sought additional resources for teaching. Student project ideas, and adaptable examples were the most popular.

Using LAMMPS for education

PRO

- Open source (GPL) = free
- No coding necessary
- Large body of potentials
- Powerful and flexible
- High student return on investment
- Established user community
- Available for Linux, Mac OS X, and now Windows binary

CON

- No GUI, or visualization
- No version control
- Significant startup investment for faculty – materials development
- Significant startup investment for students – compile and link

Discussion

- Interest level? Is there a critical mass to proceed?
- Is this a good direction for LAMMPS?
- Where to start? What is the role of Sandia staff?
  What is the role of LAMMPS users & faculty?
- Particularly interested? Email - jlane@sandia.gov