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Sandia National Laboratories

General LAMMPS Overview

Aidan Thompson, Dept. 1444, Multiscale Science
Sandia National Laboratories

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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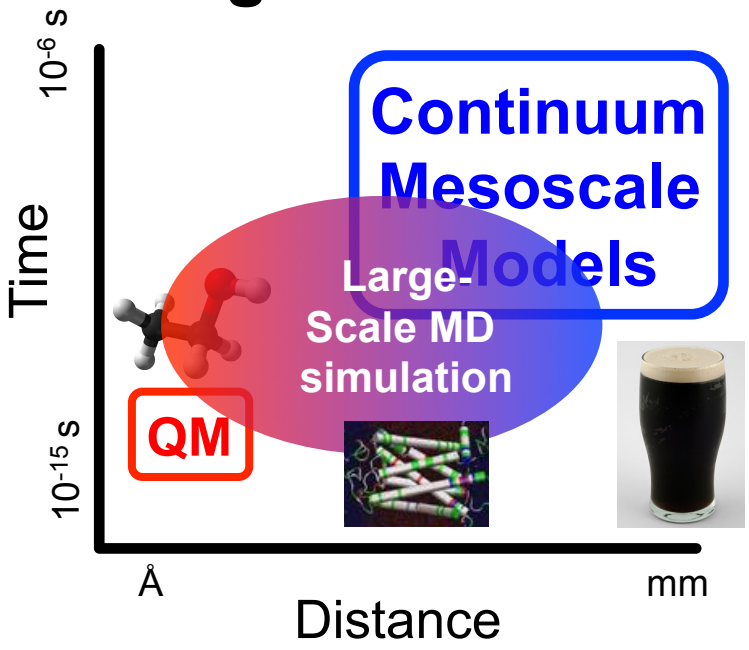
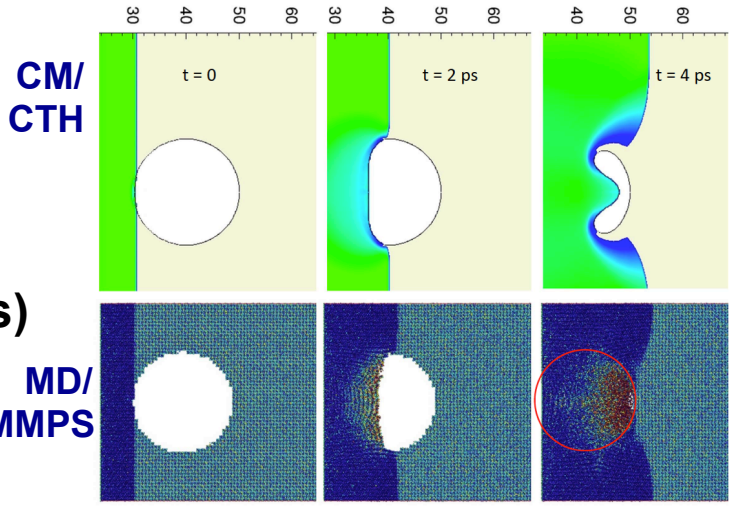
Introduction: What is large-scale MD good for?

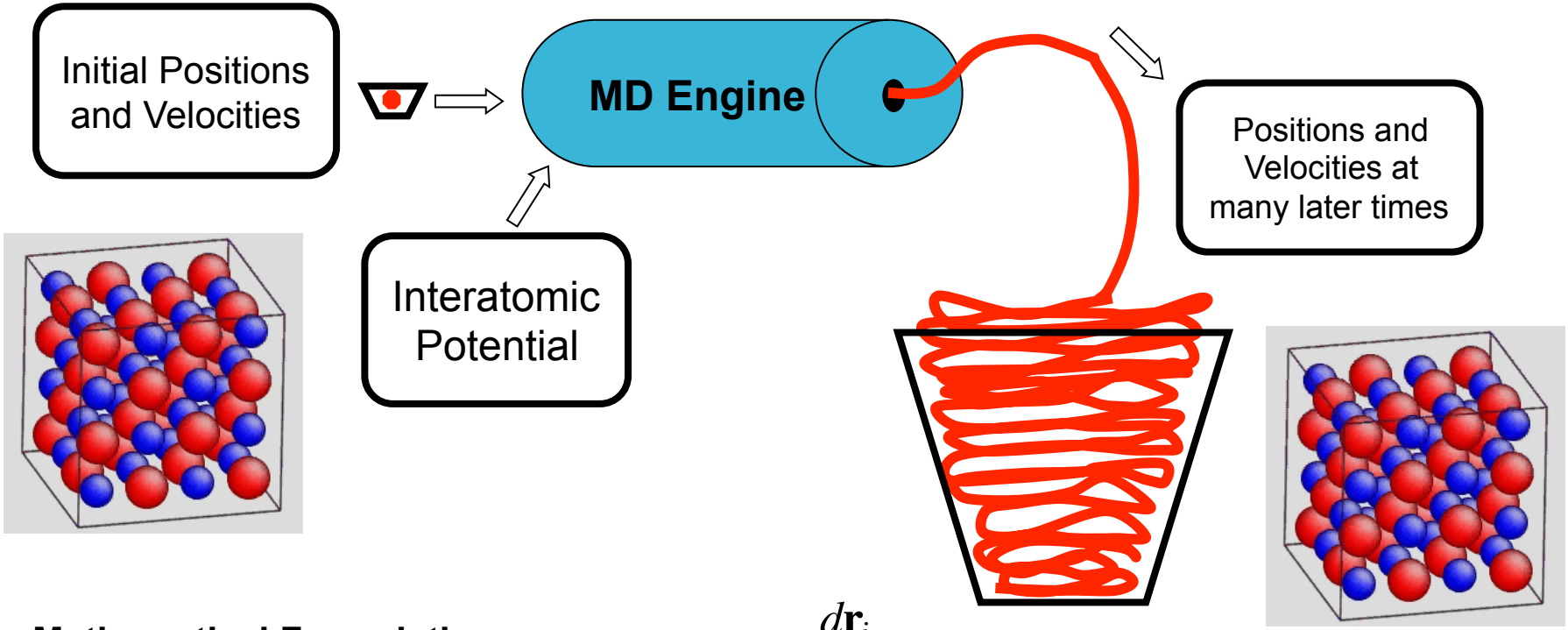
- Quantum mechanical electronic structure calculations (QM) provide accurate description of mechanical and chemical changes on the atom-scale: 10x10x10~1000 atoms
- Atom-scale phenomena drive a lot of interesting physics, chemistry, materials science, mechanics, biology…but it usually plays out on a much larger scale
- Mesoscale: much bigger than an atom, much smaller than a glass of beer.
- QM and continuum/mesoscale models (CM) can not be directly compared.
- **Small molecular dynamics (MD) simulations can be directly compared to QM results, and made to reproduce them**
- **MD can also be scaled up to millions (billions) of atoms, overlapping the low-end of CM**
- **Limitations of MD orthogonal to CM**
- **Enables us to inform CM models with quantum-accurate results**





CTH images courtesy of David Damm, Sandia

MD: What is it?



Mathematical Formulation

- Classical Mechanics
- Atoms are Point Masses: $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, ... $\boldsymbol{r}_N$
- Positions, Velocities, Forces: $\boldsymbol{r}_i$, $\boldsymbol{v}_i$, $\boldsymbol{F}_i$
- Potential Energy Function = $V(\boldsymbol{r}^N)$
- $6N$ coupled ODEs

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i$$

$$\frac{d\mathbf{v}_i}{dt} = \frac{\mathbf{F}_i}{m_i}$$

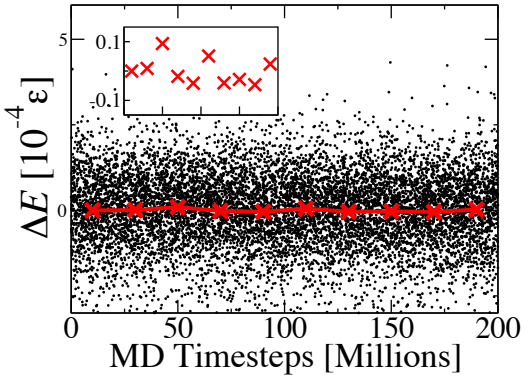
$$\mathbf{F}_i = -\frac{d}{d\mathbf{r}_i} V\left(\mathbf{r}^N\right)$$

MD Time Integration Algorithm

- Most codes and applications use variations and extensions to the Størmer-Verlet explicit integrator:

$$
\begin{aligned}
&For\ istep < nsteps: \\
&\quad \mathbf{v} \leftarrow \mathbf{v} + \frac{\Delta t}{2}\mathbf{F} \\
&\quad \mathbf{x} \leftarrow \mathbf{x} + \Delta t\,\mathbf{v} \\
&\quad Compute\ \mathbf{F}(\mathbf{x}) \\
&\quad \mathbf{v} \leftarrow \mathbf{v} + \frac{\Delta t}{2}\mathbf{F}
\end{aligned}
$$

32 atom LJ cluster,
200 million MD steps,
Δt=0.005, T=0.4



- Only second-order : $\delta E = |\langle E \rangle - E_0| \sim \Delta t^2$, but….
- ….**time-reversible, symplectic map**: global stability trumps local accuracy of high-order schemes
- More specifically, it can be shown that for Hamiltonian equations of motion, Størmer-Verlet exactly conserves a "shadow" Hamiltonian and $E-E_S \sim O(\Delta t^2)$
- For users: no energy drift over millions of timesteps
- For developers: easy to decouple integration scheme from efficient algorithms for force evaluation, parallelization.

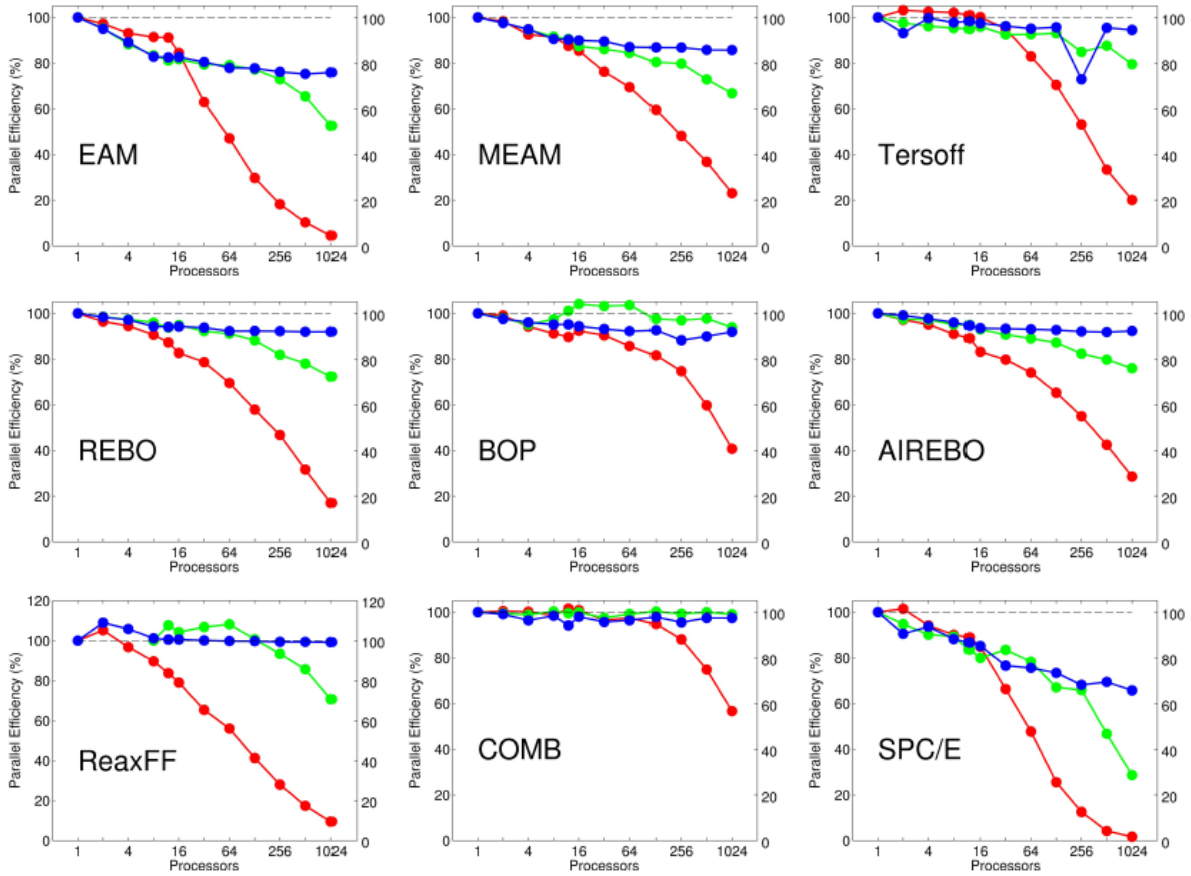
Freely Available Parallel MD Codes

- **CHARMM, AMBER:** grand-daddies of MD codes, lots of bio features
- **NAMD:** bio, clever decomposition, very scalable
- **GROMACS:** bio, fastest single processor performance, now scalable
- **DL-POLY:** soft-materials
- **GULP**: crystalline inorganic solids
- **HOOMD:** GPU-based code, fastest on single GPUs

- **LAMMPS**
  - materials oriented, wide range of interatomic potentials
  - many coarse-grained models for mesoscale to continuum
  - scalable for large simulations (1000s of particles/processor)
  - easy to extend

Why Use LAMMPS?

Answer 1: Good parallel performance



Red = 32k atoms
small fixed-size
strong scaling

Green = 1M atoms
large fixed-size
strong scaling

Blue = 32k atoms/proc
scaled size
weak scaling

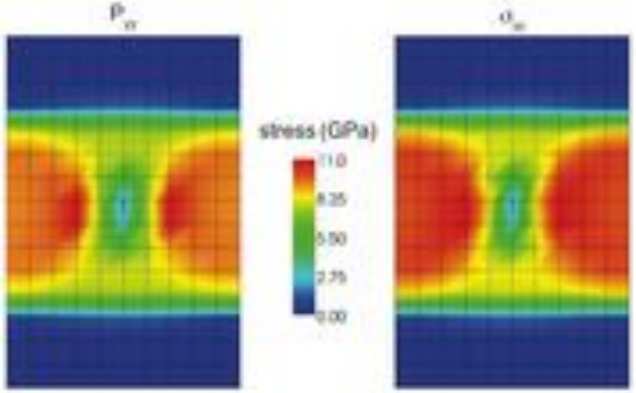
Figure 1: *Performance of 8 many-body potentials and an SPC/E water potential on varying numbers of cores of a Cray XT5 machine, as implemented in LAMMPS. For each potential, efficiency is defined as the one-processor timing divided by the P-processor timing, multiplied by 100/P. The red curves are for 32K atom systems, the green curves are for 1M atom systems; the blue curves are for scaled systems with 32K atoms per processor. The single-core CPU times per-atom per-timestep are listed in Table I.*

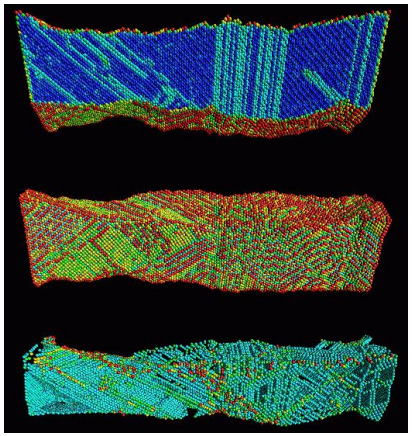
MRS Bulletin,
May 2012,
37, 513-521.

Why Use LAMMPS?

Answer 2: Versatility

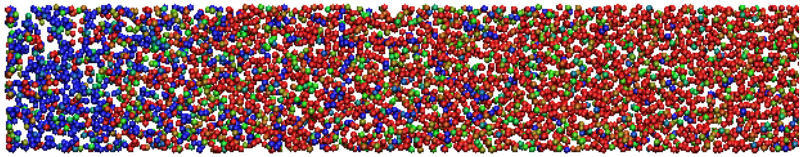
Solid Mechanics



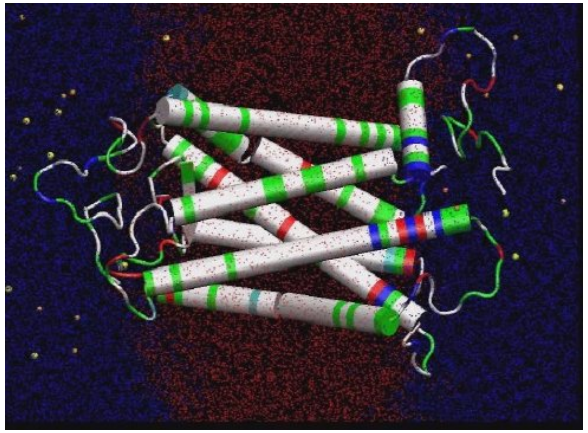


Materials Science

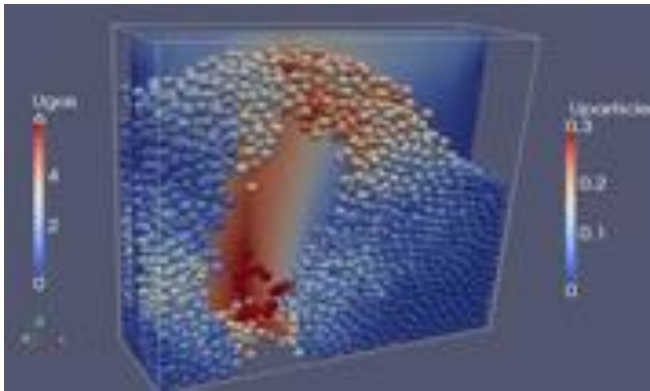
Biophysics



Chemistry



Granular Flow



Why Use LAMMPS?

Answer 3: Modularity

LAMMPS Objects

atom styles: atom, charge, colloid, ellipsoid, point dipole

pair styles: LJ, Coulomb, Tersoff, ReaxFF, AI-REBO, COMB, MEAM, EAM, Stillinger-Weber,

fix styles: NVE dynamics, Nose-Hoover, Berendsen, Langevin, SLLOD, Indentation,...

compute styles: temperatures, pressures, per-atom energy, pair correlation function, mean square displacements, spatial and time averages

Goal: All computes works with all fixes work with all pair styles work with all atom styles

Why Use LAMMPS?

Answer 4: Potential Coverage

LAMMPS Potentials by Material

Biomolecules: CHARMM, AMBER, OPLS, COMPASS (class 2), long-range Coulombics via PPPM, point dipoles, ...

Polymers: all-atom, united-atom, coarse-grain (bead-spring FENE), bond-breaking, …

Materials: EAM and MEAM for metals, Buckingham, Morse, Yukawa, Stillinger-Weber, Tersoff, COMB, SNAP, ...

Chemistry: AI-REBO, REBO, ReaxFF, eFF

Mesoscale: granular, DPD, Gay-Berne, colloidal, peri-dynamics, DSMC...

Hybrid: can use combinations of potentials for hybrid systems: water on metal, polymers/semiconductor interface, colloids in solution, …

Why Use LAMMPS?

Answer 4: Potential Coverage (contd.)

LAMMPS Potentials by Functional Form

pairwise potentials: Lennard-Jones, Buckingham, ...

charged pairwise potentials: Coulombic, point-dipole

manybody potentials: EAM, Finnis/Sinclair, modified EAM (MEAM), embedded ion (EIM), Stillinger-Weber, Tersoff, AI-REBO, ReaxFF, COMB

coarse-grained potentials: DPD, GayBerne, ...

mesoscopic potentials: granular, peridynamics

long-range electrostatics: Ewald, PPPM, MSM

implicit solvent potentials: hydrodynamic lubrication, Debye

force-field compatibility with common CHARMM, AMBER, OPLS, GROMACS options

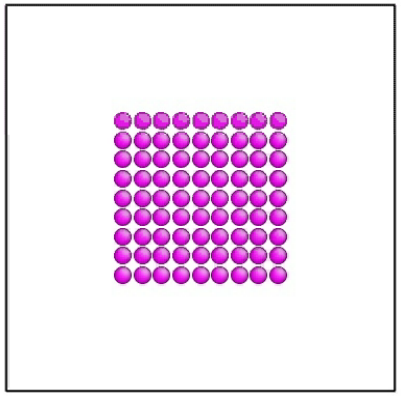
Why Use LAMMPS?

Answer 5: Easily extensible

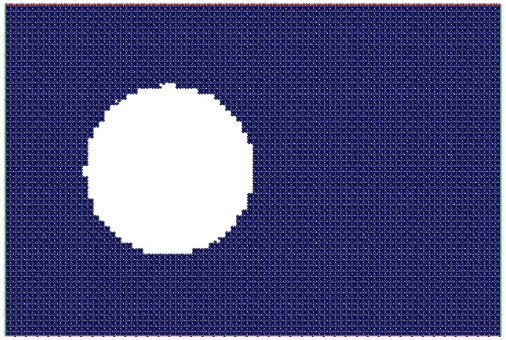
- **One of the best features of LAMMPS**
  - 90% of code is “extensions” via styles
  - only ~35K of 474K lines is core of LAMMPS
- **Easy to add new features via 14 “styles”**
  - new particle types = atom style
  - new force fields = pair style, bond style, angle style, dihedral style, improper style
  - new long range = kspace style
  - new minimizer = min style
  - new geometric region = region style
  - new output = dump style
  - new integrator = integrate style
  - new computations = compute style (global, per-atom, local)
  - new fix = fix style = BC, constraint, time integration, ...
  - new input command = command style = read_data, velocity, run, …
- **Enabled by C++**
  - virtual parent class for all styles, e.g. pair potentials
  - defines interface the feature must provide
  - compute(), init(), coeff(), restart(), etc

Why Use LAMMPS?

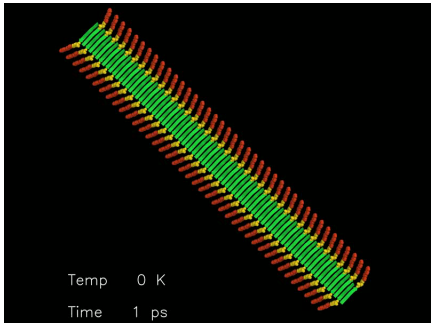
Answer 6: Movies



This is work by Aidan Thompson at home on his couch. It demonstrates an ordered solid cluster undergoing a melting transition to form a liquid droplet in equilibrium with a confined vapor phase. It provides a very direct demonstration of why there are three “states of matter.”



This is work by Ray Shan and Aidan Thompson at Sandia National Laboratories showing a 2 km/s shockwave passing through a spherical void in a molecular crystal of PETN. The shockwave produces a jet at the void surface which collides with the opposite surface. The collision creates a local hotspot, elevated temperature, chemical reaction, leading to initiation of detonation.



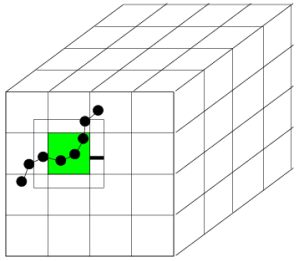
This is work by Alexey Shaytan et al. at the Dept of Energy-Related Nanomaterials (University of Ulm, Germany) on a large-scale fully atomistic MD simulation of the amyloid-like nanofibers formed by the conjugates of oligothiophenes and oligopeptides. Such compounds are very promising for applications in organic electronics (conductive organic nanowires).

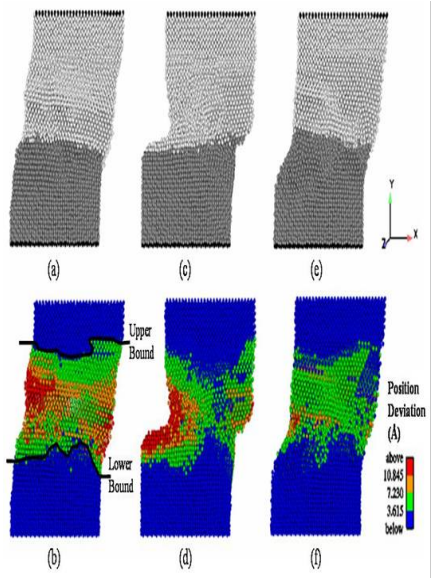
BACKUP

What is LAMMPS?

(Large-scale Atomic/Molecular Massively Parallel Simulator)

http://lammps.sandia.gov





- Classical MD code.
- Open source, highly portable C++.
- Freely available for download under GPL.
- Easy to download, install, and run.
- Well documented.
- Easy to modify or extend with new features and functionality.
- Active users e-mail list with over **650** subscribers.
- Users' workshops: February 2010, August 2011, August 2013.
- Spatial-decomposition of simulation domain for parallelism.
- Energy minimization via conjugate-gradient relaxation.
- Atomistic, mesoscale, and coarse-grain simulations.
- Variety of potentials (including many-body and coarse-grain).
- Variety of boundary conditions, constraints, etc.