SAND2010-1221C

LAMMPS for Computational Material Science Research and Education

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Albuquerque, NM

15/16 February 2010

Integrated Computational Materials Research & Education Roundtable

TMS Annual Meeting, Seattle, WA

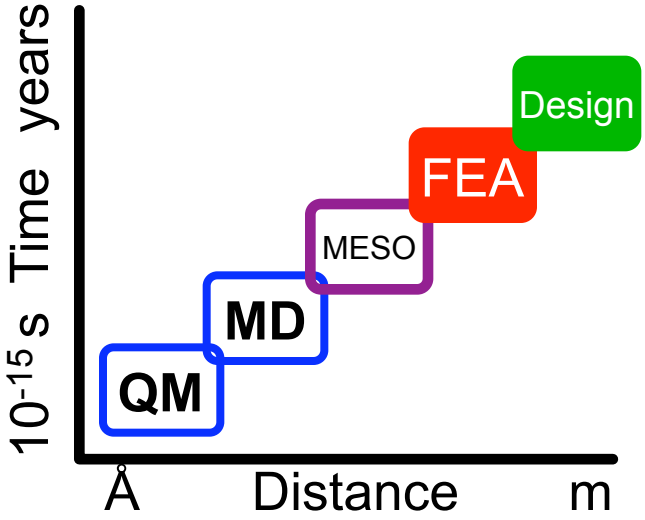
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

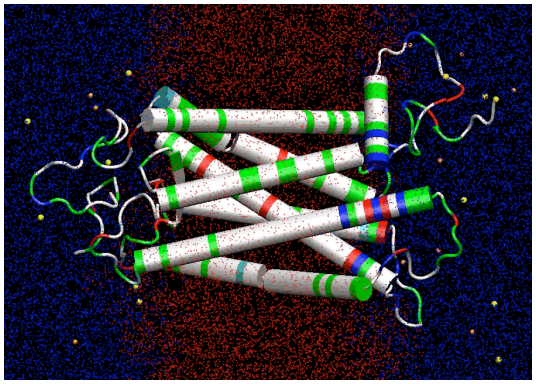
LAMMPS scope and examples

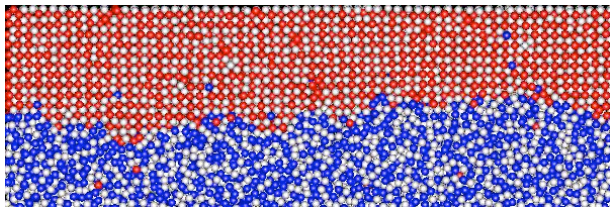
Large-scale **A**tomic/**M**olecular **M**assively **P**arallel **S**imulator

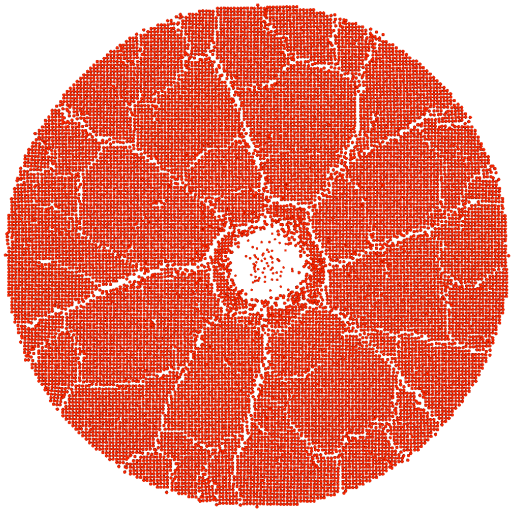
Three primary communities are supported by force fields, boundary conditions and diagnostics:

- biomolecules and polymers (soft materials)
- materials science (solids)
- mesoscale to continuum









Molecular Dynamics (MD) simulations

- Solve Newton's equation…

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{F}_i$$

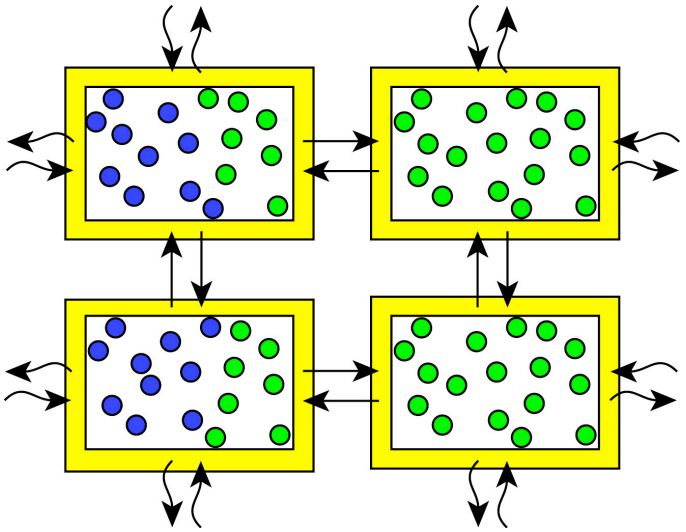
$$\mathbf{F}_i = -\nabla V_i$$

6*N* coupled ODEs

$$\begin{aligned}
\mathbf{v}_i^{(l+\frac{1}{2})} &= \mathbf{v}_i^l - \frac{\mathbf{F}_i^l}{2m_i}\Delta t \\
\mathbf{r}_i^{(l+1)} &= \mathbf{r}_i^l + \mathbf{v}_i^{(l+\frac{1}{2})}\Delta t \\
\mathbf{v}_i^{(l+1)} &= \mathbf{v}_i^{(l+\frac{1}{2})} - \frac{\mathbf{F}_i^{(l+1)}}{2m_i}\Delta t
\end{aligned}$$

Mathematical Formulation

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



Sandia's LAMMPS code is spatially parallel

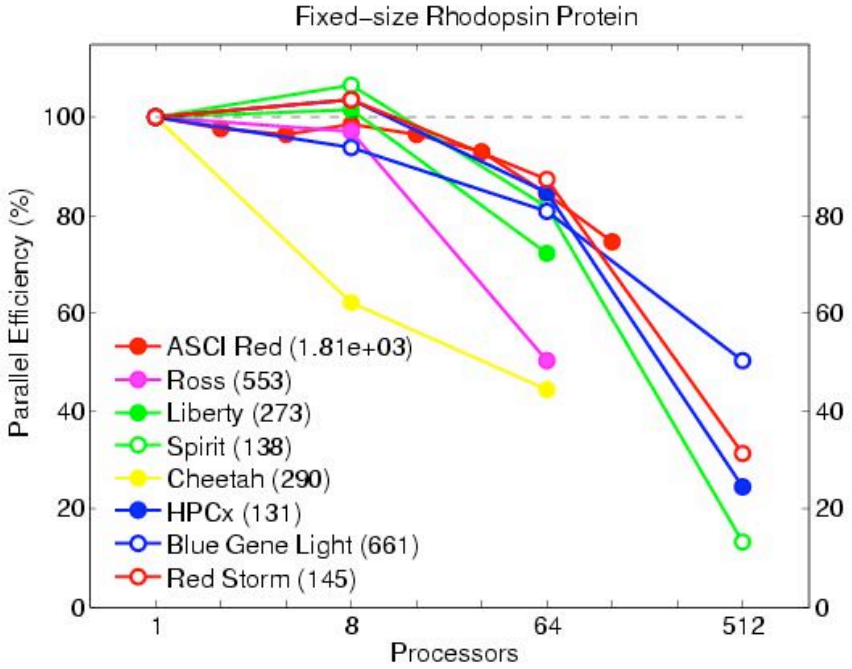
Large-scale **A**tomic/**M**olecular **M**assively **P**arallel **S**imulator

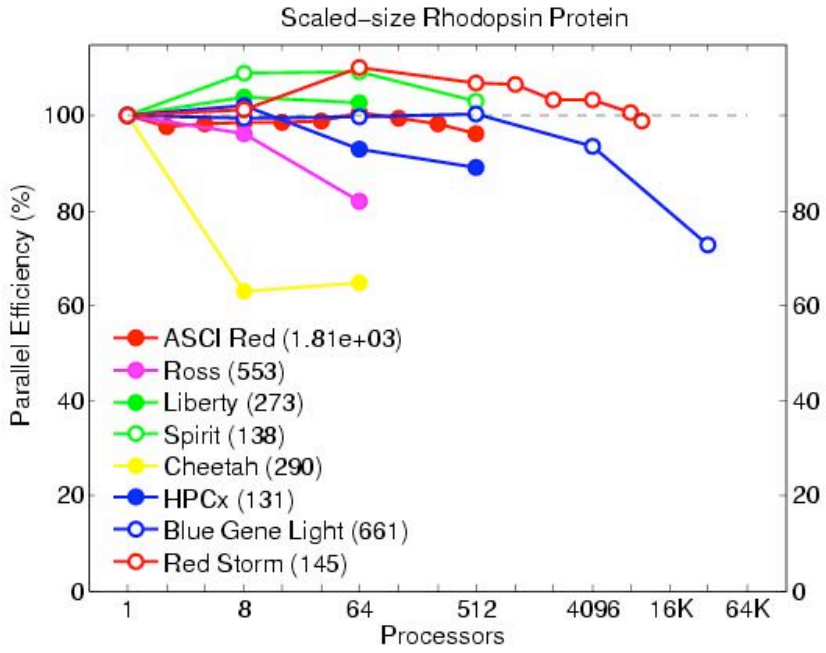
Problem: Δt tied to the fastest atomic motion t is the timescale of physical interest

$nsteps = t / \Delta t = 10^6 \ldots 10^{15}$

LAMMPS scaling performance

- **Fixed-size (32K atoms) & scaled-size (32K/proc) parallel efficiencies**
- **Protein (rhodopsin) in solvated lipid bilayer**





- **Billions of atoms on 64K procs of Blue Gene or Red Storm**
- **Opteron speed: 4.5E-5 sec/atom/step (12x for metal, 25x for LJ)**

Wide variety of pre-coded force fields

Biomolecules:

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

Polymers:

all-atom, united-atom, bead-spring FENE, bond-breaking, bond-forming, ...

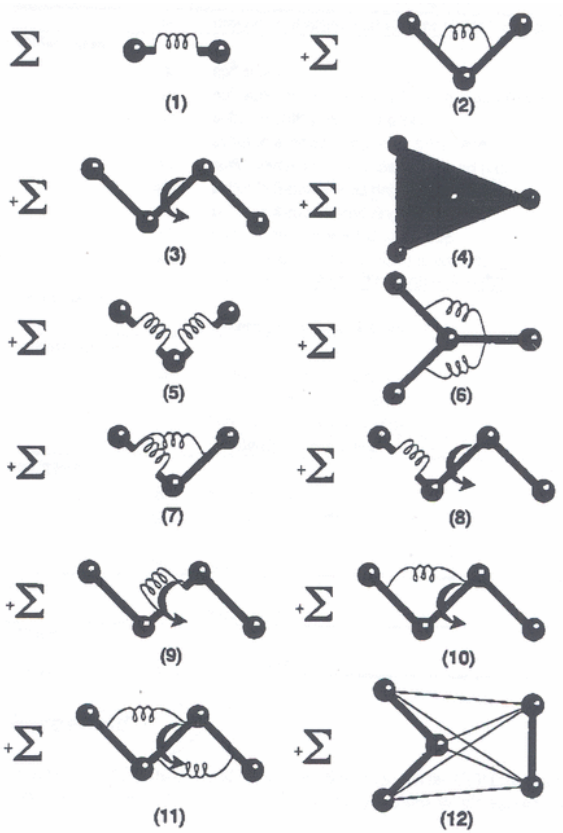
Materials:

EAM/MEAM for metals, Buckingham, Morse, Yukawa, Stillinger-Weber, Tersoff, AI-REBO, REAXX, ...

Mesoscale:

granular, DPD, SPH, DSMC, PD, MPM, ...

$$E = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad r < r_c$$



What LAMMPS is and is not

- MD engine for atoms/molecules/ particles at any length/time scale
  - particle interactions via neighbor lists
  - integrate Newton's equations
- 120K lines of portable C++
  - C++ for top-level objects
  - C-style coding and data structures underneath
- Open source (GPL)
- Limited support for pre-processing
  - No molecular builders
- Limited on-the-fly diagnostics
  - Users add modules to do this
- Limited support for post-processing
  - No GUI, or visualization
- Good external codes are avalable:
  - pre- and post-processing codes distributed with LAMMPS
  - Pizza.py toolkit of Python tools
  - LAMMPS formats are readable by many visualization codes

Learning more about LAMMPS

- Very active website ~ http://lammps.sandia.gov
  - documentation, pictures, movies, publications
  - new releases twice per year, continuous patches
- Examples directory
- Large user community and listserve
- Increased interest in educational materials for faculty