



# LAMMPS Workshop

## General Introduction

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Physics Department  
Sharif University of Technology  
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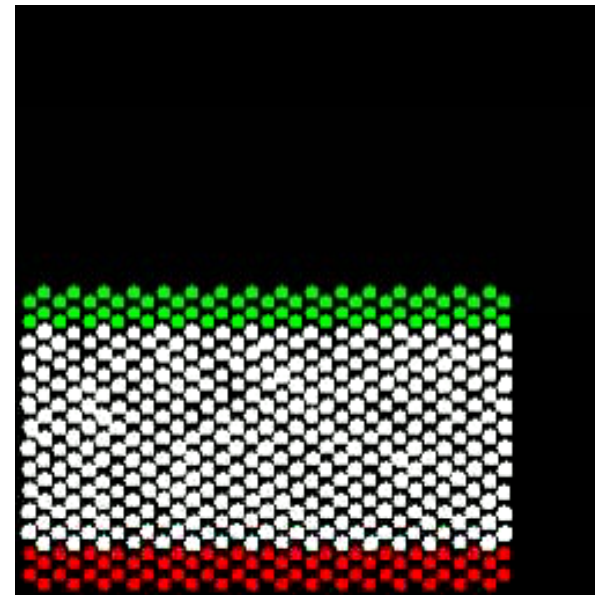
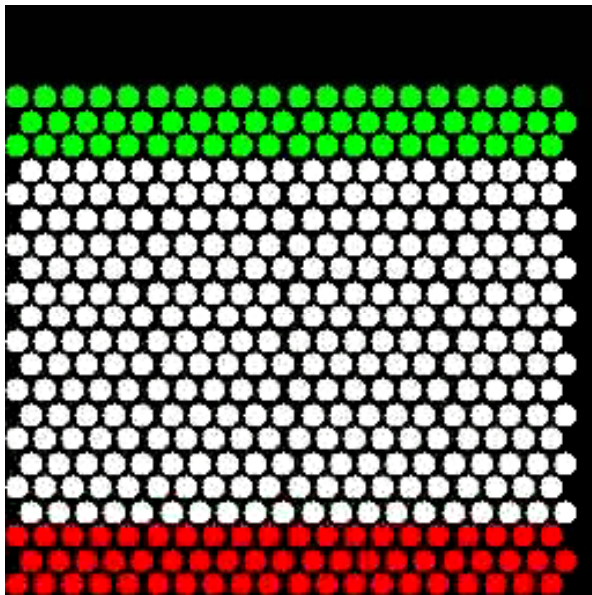


# Contents

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- 
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# What is LAMMPS

- **L**arge-scale **A**tomic/**M**olecular **M**assively **P**arallel **S**imulator
- A *classical* molecular dynamics code
- models an ensemble of particles in a *gaseous, liquid or solid state*



# What is LAMMPS (Cont.)

- LAMMPS is a freely-available *open-source* code, distributed under the terms of the GNU Public License (GPL)

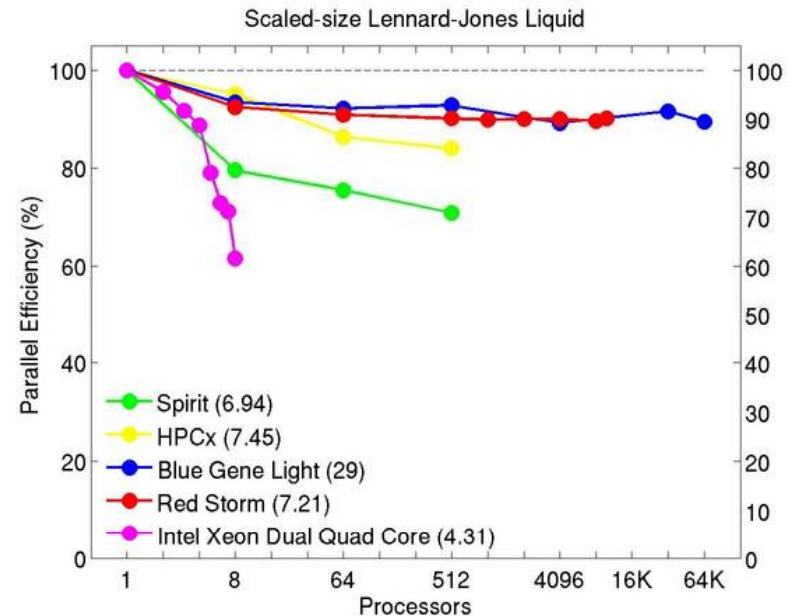
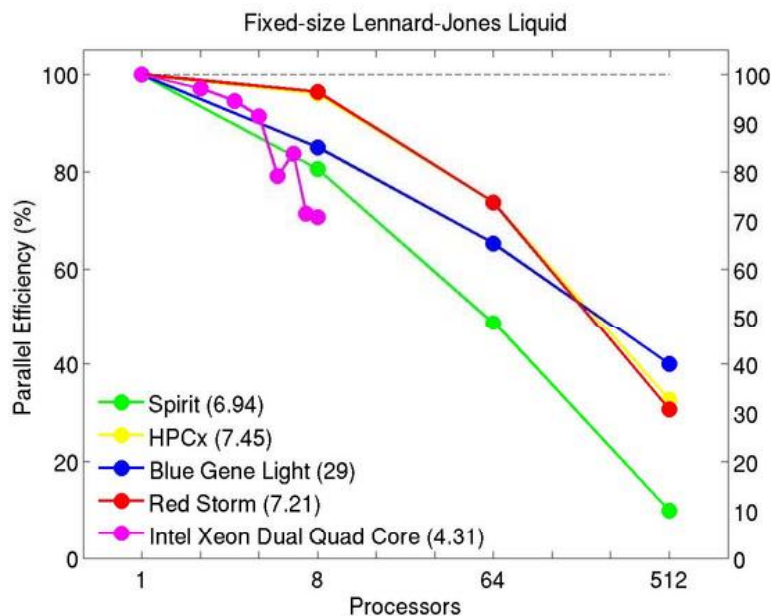


- Developed at Sandia National Laboratories, a US Department of Energy facility, with funding from the DOE



# General Features

- Runs on a single processor or in parallel distributed-memory message-passing parallelism (MPI)
- Spatial-decomposition of simulation domain for parallelism
- Can model systems with only a few particles up to millions or billions





## General Features (Cont.)

- Designed to be easy to modify or extend with new capabilities, such as:
  - force fields,
  - atom types,
  - boundary conditions.
- The current version of LAMMPS is written in C++. Earlier versions were written in F77 and F90.



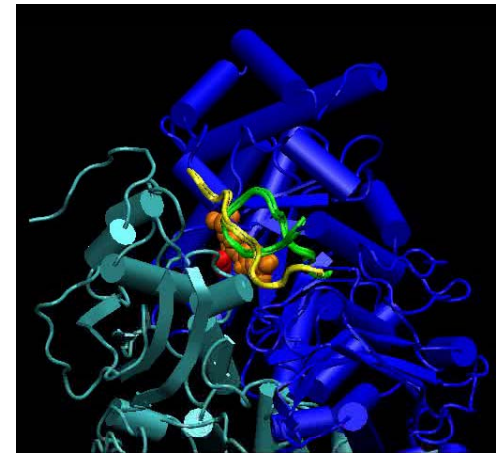
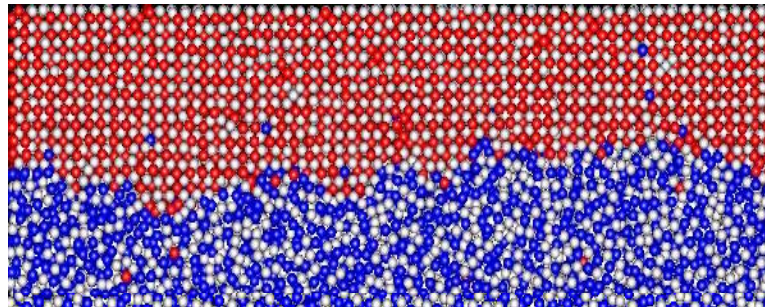
## General Features (Cont.)

- Runs from an input script
  - Syntax for defining and using variables and formulas
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- Syntax for looping over runs and breaking out of loops
  - Run one or multiple simulations simultaneously (in parallel) from one script



# Kinds of Systems LAMMPS Can Simulate

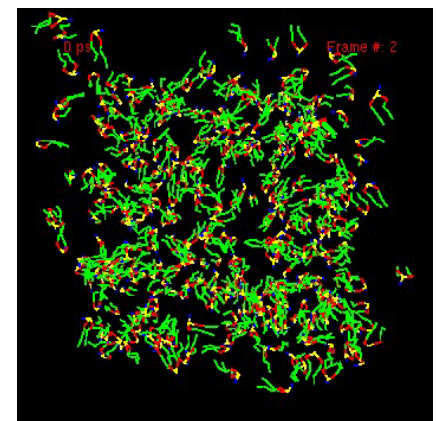
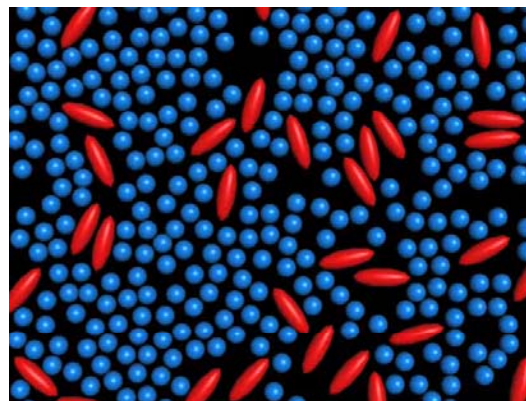
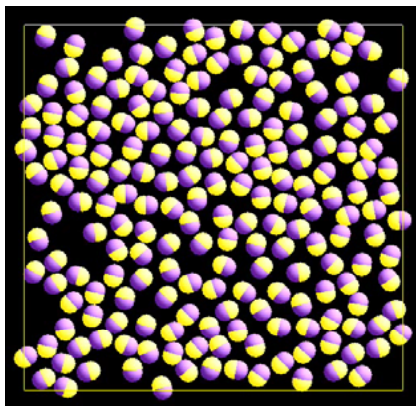
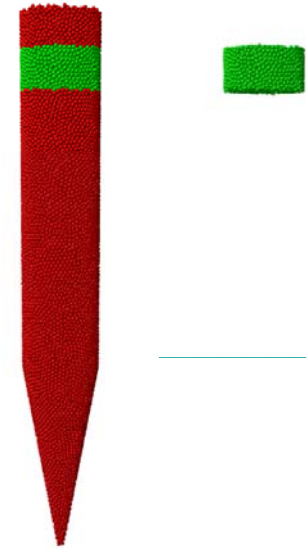
- atomic (e.g. box of Lennard-Jonesium)
- bead-spring polymers
- united-atom polymers or organic molecules
- all-atom polymers, organic molecules, proteins, DNA
- metals





# Kinds of systems LAMMPS Can Simulate (Cont.)

- granular materials
- coarse-grained mesoscale models
- ellipsoidal particles
- point dipolar particles
- **hybrid combinations of these**



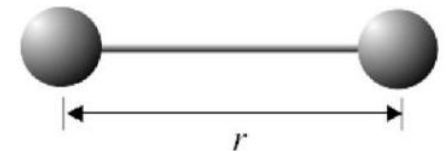


# Creation of Atoms

- Read in atom coordinates from files
- Create atoms on one or more lattices (e.g. grain boundaries)
- Delete geometric or logical groups of atoms (e.g. voids)
- Displace atoms

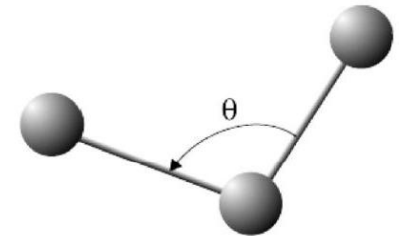
# Force Fields

- **Pair wise potentials:** Lennard-Jones, Buckingham, Morse, Yukawa, soft, class 2 (COMPASS), tabulated
- **Charged pair wise potentials:** Coulombic, point-dipole
- **Many body potentials:** EAM, Finnis/Sinclair EAM, modified EAM (MEAM), Stillinger-Weber, Tersoff, AI-REBO, ReaxFF
- **Coarse-grain potentials:** DPD, GayBerne, REsquared, colloidal
- **Mesosopic potentials:** granular, Peridynamics
- **Bond potentials:** harmonic, FENE, Morse, nonlinear, class 2, quartic (breakable)

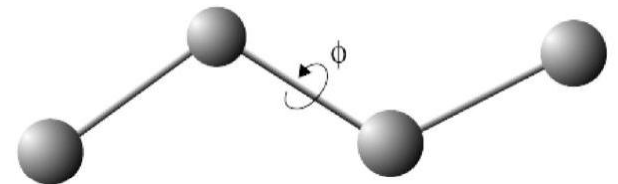


# Force Fields (Cont.)

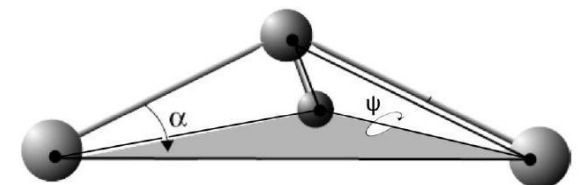
- **Angle potentials:** harmonic, CHARMM, cosine, cosine/squared, class 2 (COMPASS)



- **Dihedral potentials:** harmonic, CHARMM, multi-harmonic, helix, class 2 (COMPASS), OPLS



- **Improper potentials:** harmonic, cvff, class 2 (COMPASS)



- **Hybrid potentials:** multiple pair, bond, angle, dihedral, improper potentials can be used in one simulation



## Force Fields (Cont.)

- **Polymer potentials:** all-atom, united-atom, bead-spring, breakable
- **Explicit Water potentials:** TIP3P, TIP4P, SPC
- **Implicit solvent potentials:** hydrodynamic lubrication, Debye
- **Long-range** Coulombics and dispersion: Ewald, PPPM (similar to particle-mesh Ewald)



# Ensembles, constraints, and boundary conditions

- 2D or 3D systems
  - Constant NVE, NVT, NPT, NPH integrators
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- Thermostatting options for groups and geometric regions of atoms
  - Pressure control via Nose/Hoover or Berendsen barostatting in 1 to 3 dimensions



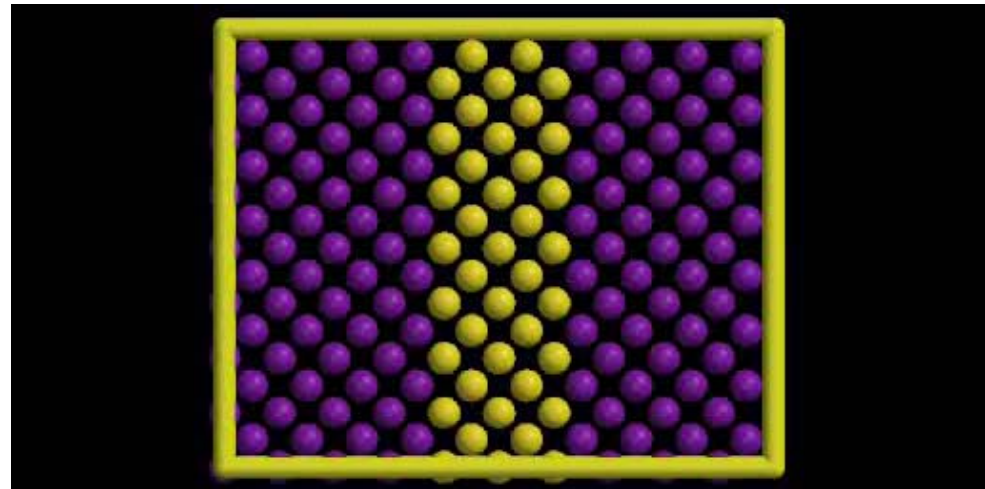


## Ensembles, constraints, and boundary conditions (Cont.)

- Simulation box deformation (tensile and shear)
- Harmonic (umbrella) constraint forces
- SHAKE bond and angle constraints

# Ensembles, constraints, and boundary conditions (Cont.)

- targeted molecular dynamics (TMD) and steered molecule dynamics (SMD) constraints
- non-equilibrium molecular dynamics (NEMD)
- variety of additional boundary conditions and constraints





# Integrators

- Velocity-Verlet integrator
  - Brownian dynamics
- 
- Energy minimization via:
    - conjugate gradient
    - steepest descent
  - r-RESPA hierarchical time stepping



# Output

- Log file of thermodynamic info
  - Text dump files of atom coords, velocities, other per-atom quantities
- 
- Binary restart files
  - Output formats: native, XYZ, XTC, DCD



# LAMMPS Specialized Features

- real-time visualization and interactive MD
  - atom-to-continuum coupling with finite elements
- 
- parallel tempering
  - parallel replica dynamics
  - Direct Simulation Monte Carlo for low-density fluids
  - Peridynamics mesoscale modeling
  - targeted and steered molecular dynamics



# LAMMPS Non-Features

- Specifically, LAMMPS itself does not:
    - GUI
    - build molecular systems
    - assign force-field coefficients automatically
    - perform sophisticated analyses of your MD simulation
    - visualize your MD simulation
    - plot your output data
-





# LAMMPS Non-Features (Cont.)

- Reasons:
    - the desire to keep LAMMPS simple
    - they are not parallel operations
    - other codes already do them
-



# Pre- and Post-Processing

- A separate toolkit called *Pizza*
- *Pizza* provides tools for doing:
  - setup
  - analysis
  - plotting
  - visualizationfor LAMMPS simulations
- *Pizza* is written in Python



# LAMMPS vs. Other Codes

- CHARMM, AMBER, NAMD, NWCHEM, and Tinker are designed primarily for modeling biological molecules
- CHARMM and AMBER use atom-decomposition (replicated-data) strategies for parallelism.
- NAMD and NWCHEM use spatial-decomposition approaches, similar to LAMMPS.
- Tinker is a serial code.
- CHARMM is commercial
- NAMD can not use Implicit solvents.



# LAMMPS vs. GROMACS

- GROMACS:
  - is easier to use and specified for biological molecules.
  - more water explicit models
  - more post processing utilities.
  - LAMMPS only support SHAKE constraint
- LAMPPS do more simulation tasks:
  - Implicit solvent
  - More systems: granular materials, coarse-grained mesoscale models, ellipsoidal particles



# References

- <http://lammps.sandia.gov/>
  - <http://lammps.sandia.gov/doc/Manual.html>
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- Thank you for your attention.
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