# A Quick Tour of LAMMPS

Steve Plimpton
Sandia National Labs
sjplimp@sandia.gov

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Follow along with my slides at:
http://lammps.sandia.gov/workshops/Aug17/workshop.html

**CCR**
Center for Computing Research

Sandia
National
Laboratories

National Nuclear Security Administration

# Resources for learning LAMMPS

All on web site, most in distro tarball:

- Workshops (beginner tutorials), Tutorials
- Features: list of features with links
- Glossary: MD terms $\Rightarrow$ LAMMPS
- Manual:
    - Intro, Commands, Packages, Accelerating, Howto, Modifying, Errors sections
    - search bubble at top left of every page
- Commands
    - alphabetized command & style tables: one page per command
- Papers: find a paper similar to what you want to model
- Mail list: search archives (lammps-users, post Qs to it
    - http://lammps.sandia.gov/mail.html
- Examples: 50 sub-dirs under examples in distro
    - lower-case = simple, upper-case = more complex
    - many produce movies: http://lammps.sandia.gov/movies.html

# Structure of typical input scripts

1. Units and atom style
2. Create simulation box and atoms
   - region, create_box, create_atoms, region commands
     - lattice command vs box units
   - read_data command
     - data file is a text file
     - look at examples/micelle/data.micelle
     - see read_data doc page for full syntax
3. Define groups
4. Set attributes of atoms: mass, velocity
5. Pair style for atom interactions
6. Fixes for time integration and constraints
7. Computes for diagnostics
8. Output: thermo, dump, restart
9. Run or minimize
10. Rinse and repeat (script executed one command at a time)

# Obstacle example

input script = examples/obstacle/in.obstacle
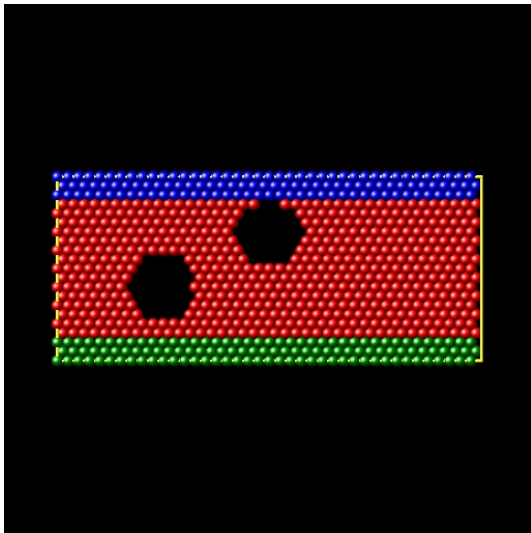
# Obstacle input script

1st section = setup box and create atoms

```
# 2d LJ obstacle flow

dimension 2
boundary p s p
atom_style atomic
neighbor 0.3 bin
neigh_modify delay 5

# create geometry

lattice hex 0.7
region box block 0 40 0 10 -0.25 0.25
create_box 3 box
create_atoms 1 box
```

# Obstacle input script

2nd section = define potential and groups of atoms

```
# LJ potentials

pair_style lj/cut 1.12246
pair_coeff * * 1.0 1.0 1.12246

# define groups

region 1 block INF INF INF 1.25 INF INF
group lower region 1
region 2 block INF INF 8.75 INF INF INF
group upper region 2
group boundary union lower upper
group flow subtract all boundary

set group lower type 2
set group upper type 3
```

# Obstacle input script

3rd section = set velocities and fixes

```
# initial velocities

mass * 1.0
compute mobile flow temp
velocity flow create 1.0 482748 temp mobile
fix 1 all nve
fix 2 flow temp/rescale 200 1.0 1.0 0.02 1.0
fix_modify 2 temp mobile

# Poiseuille flow

velocity boundary set 0.0 0.0 0.0
fix 3 lower setforce 0.0 0.0 0.0
fix 4 upper setforce 0.0 NULL 0.0
fix 5 upper aveforce 0.0 -0.5 0.0
fix 6 flow addforce 1.0 0.0 0.0
```

# Obstacle input script

4th section = create 2 obstacles to flow

```
# 2 obstacles

region void1 sphere 10 4 0 3
delete_atoms region void1
region void2 sphere 20 7 0 3
delete_atoms region void2

fix 7 flow indent 100 sphere 10 4 0 4
fix 8 flow indent 100 sphere 20 7 0 4
fix 9 all enforce2d
```

# Obstacle input script

5th section: define output and run simulation (JPG, PNG, PPM)

```
# run

timestep 0.003
thermo 1000
thermo_modify temp mobile

#dump 1 all atom 100 dump.obstacle
dump 1 all image 500 image.*.ppm type type &
zoom 1.6 adiam 1.5
dump_modify 1 pad 5

run 25000
```

# Obstacle example

Questions on input script?

Exercise:
    run examples/obstacle/in.obstacle on your box
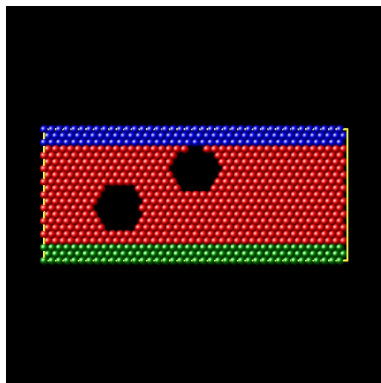    examine output

# Make a movie

**50 JPG or PNG or PPM files**

- image.16500.jpg
- ImageMagick display
- Mac Preview

**Make/view a movie**

- ImageMagick
  convert *.jpg image.gif
- open in browser
  open -a Safari image.gif
- Mac QuickTime
  open image sequence
- Windows Media Player
- Ovito, VMD, AtomEye, ...
- Breakout session on Ovito

# Examine screen output

```
LAMMPS (15 Aug 2013)
Lattice spacing in x,y,z = 1.28436 2.22457 1.28436
Created orthogonal box = (0 0 -0.321089)
              to (51.3743 22.2457 0.321089)
  4 by 1 by 1 MPI processor grid
Created 840 atoms
120 atoms in group lower
120 atoms in group upper
240 atoms in group boundary
600 atoms in group flow
Setting atom values ...
  120 settings made for type
Setting atom values ...
  120 settings made for type
Deleted 36 atoms, new total = 804
Deleted 35 atoms, new total = 769
```

# Thermo output

```
Setting up run ...
Memory usage per processor = 2.23494 Mbytes
Step Temp E_pair E_mol TotEng Press Volume
0 1.0004177 0 0 0.68689281 0.46210058 1143.0857
1000 1 -0.32494012 0 0.36166587 1.2240503 1282.5239
2000 1 -0.37815616 0 0.30844982 1.0642877 1312.5691
...
...
...
25000 1 -0.36649381 0 0.32011217 0.98366691 1451.5444
25000 1 -0.38890426 0 0.29770172 0.95284427 1455.9361
Loop time of 1.76555 on 4 procs for
        25000 steps with 769 atoms
```

# Timing info

```
Loop time of 1.76555 on 4 procs for
        25000 steps with 769 atoms

Pair time (%) = 0.14617 (8.27903)
Neigh time (%) = 0.0467809 (2.64966)
Comm time (%) = 0.307951 (17.4422)
Outpt time (%) = 0.674575 (38.2078)
Other time (%) = 0.590069 (33.4213)
```

# Run statistics

Per-processor values at end of run

```
Nlocal:  192.25 ave 242 max 159 min
Histogram:  2 0 0 0 0 1 0 0 0 1
Nghost:  43 ave 45 max 39 min
Histogram:  1 0 0 0 0 0 0 0 2 1
Neighs:  414 ave 588 max 284 min
Histogram:  2 0 0 0 0 0 1 0 0 1

Total # of neighbors = 1656
Ave neighs/atom = 2.15345
Neighbor list builds = 1641
Dangerous builds = 1
```

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Questions on output?

# Defining variables in input scripts

- **Styles**: index, loop, equal, atom, ...
  - variable x index run1 run2 run3 run4
  - variable x loop 100
  - variable x trap(f_JJ[3])*${scale}
  - variable x atom -(c_p[1]+c_p[2]+c_p[3])/(3*vol)

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  - variable x trap(f_JJ[3])*${scale}
  - variable x atom -(c_p[1]+c_p[2]+c_p[3])/(3*vol)
- **Formulas** can be complex
  - see doc/variable.html
  - thermo keywords (temp, press, ...)
  - math operators & functions (sqrt, log, cos, ...)
  - group and region functions (count, xcm, fcm, ...)
  - various special functions (min, ave, trap, stride, stagger, ...)
  - per-atom vectors (x, vx, fx, ...)
  - output from computes, fixes, other variables
- Formulas can be **time**- and/or **spatially**-dependent

# Using variables in input scripts

- Substitute in any command via $x or ${myVar}
- Immediate formula evaluation via $ syntax:
  - avoids need to define variable separately
  - variable xmid equal (xlo+xhi)/2
  - region 1 block $xmid EDGE INF INF EDGE EDGE
  - region 1 block $((xlo+xhi)/2) EDGE INF INF EDGE EDGE
- Next command increments a variable to next value
- Many commands allow variables as arguments
  - fix addforce 0.0 v_fy 1.0
  - dump_modify every v_foo
  - region sphere 0.0 0.0 0.0 v_radius

# Power tools for input scripts

- Filename options:
  - dump.*.% for per-snapshot or per-processor output
  - read_data data.protein.gz
  - read_restart old.restart.*
- If/then/else via if command
- Insert another script via include command
  - useful for long list of params

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- Filename options:
  - dump.*.% for per-snapshot or per-processor output
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- Insert another script via include command
  - useful for long list of params
- Looping via next and jump commands
- Invoke a shell command or external program
  - shell cd subdir1
  - shell my_analyze out.file $n ${param}
- (New!) Invoke Python code from your script
  - pass LAMMPS data to Python, return values in variables
  - Python function can make callbacks to LAMMPS
- Various ways to run multiple simulations from one script
  - see doc/Section_howto 6.4

# Example script for multiple runs

8 successive simulations on P processors:

```
variable r equal random(1,1000000000,58798)
variable a loop 8
variable t index 0.8 0.85 0.9 0.95 1.0 1.05 1.1 1.15
log log.$a
read data.polymer
velocity all create $t $r
fix 1 all nvt $t $t 1.0
dump 1 all atom 1000 dump.$a.*
run 100000
next t
next a
jump in.polymer
```

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variable a loop 8
variable t index 0.8 0.85 0.9 0.95 1.0 1.05 1.1 1.15
log log.$a
read data.polymer
velocity all create $t $r
fix 1 all nvt $t $t 1.0
dump 1 all atom 1000 dump.$a.*
run 100000
next t
next a
jump in.polymer
```

Run 8 simulations on 3 partitions until finished:

- change a & t to universe-style variables
- mpirun -np 12 lmp_linux -p 3x4 -in in.polymer

# Pre-processing tools to build complex systems

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- Data file must include list of bonds, angles, etc
- Data file can include force field assignments
- Tools directory has converters for both steps
  - ch2lmp = CHARMM converter
  - amber2lmp = AMBER converter
  - msi2lmp = Accelrys converter

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  - ch2lmp = CHARMM converter
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- Provided builders
  - Moltemplate (Andrew Jewett)
  - Pizza.py = chain and patch tools (Python)
- Builders that can create LAMMPS input
  - see http://lammps.sandia.gov/prepost.html
  - VMD TopoTools (Axel Kohlmeyer)
  - Avogadro, Packmol, EMC (breakout A2)

**EMC: Initial Structure Generation**
*Option A2, Thursday, 1-3pm*
*http://montecarlo.sourceforge.net/*
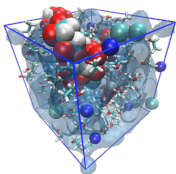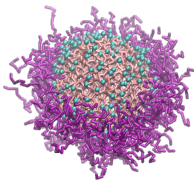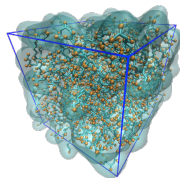


bulk        graft        copolymer
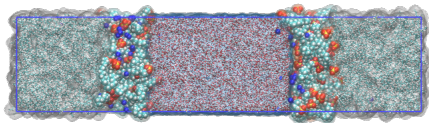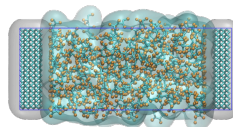
multiphase        surface

# Pair styles

LAMMPS lingo for interaction potentials

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- A pair style can be true pair-wise or many-body
  - LJ, Coulombic, Buckingham, Morse, Yukawa, ...
  - EAM, Tersoff, REBO, ReaxFF, ...
- Bond/angle/dihedral/improper styles = permanent bonds

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- Bond/angle/dihedral/improper styles = permanent bonds
- Variants optimized for GPU and many-core
  - GPU, USER-OMP, USER-INTEL, KOKKOS packages
  - lj/cut, lj/cut/gpu, lj/cut/kk, lj/cut/omp
  - see doc/Section_accelerate.html
  - see Kokkos talk by Stan Moore on Thurs AM
- Coulomb interactions included in pair style
  - lj/cut, lj/cut/coul/cut, lj/cut/coul/wolf, lj/cut/coul/long
  - done to optimize inner loop

# Categories of pair styles

- Solids
  - eam, eim, meam, adp, etc
- Bio and polymers
  - charmm, class2, gromacs, dreiding, etc
- Reactive
  - tersoff, bop, airebo, comb, reax/c, etc
- Coarse-grained
  - dpd, granular, sph, peri, colloid, lubricate, brownian, FLD
- Aspherical
  - gayberne, resquared, line, tri, etc

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- Pair table for tabulation of any pair-wise interaction
- Pair hybrid style allows for hybrid models
  - polymers on metal
  - CNTs in water
  - solid-solid interface between 2 materials

# Pair styles

See doc/Section_commands.html for full list
Annotated with (cgikot) for accelerated variants

| | | | |
|---|---|---|---|
| none | hybrid | hybrid/overlay | adp (o) |
| airebo (o) | beck (go) | body | bop |
| born (o) | born/coul/long (cgo) | born/coul/msm | born/coul/msm (o) |
| born/coul/wolf (go) | brownian (o) | brownian/poly (o) | buck (cgko) |
| buck/coul/cut (cgko) | buck/coul/long (cgko) | buck/coul/msm | buck/coul/msm (o) |
| buck/long/coul/long (o) | colloid (go) | comb (o) | comb3 |
| coul/cut (gko) | coul/debye (gko) | coul/dsf (gko) | coul/long (gko) |
| coul/long/cs | coul/msm | coul/streitz | coul/wolf (ko) |
| dpd (o) | dpd/tstat (o) | dsmc | eam (cgkot) |
| eam/alloy (cgkot) | eam/fs (cgkot) | eim (o) | gauss (go) |
| gayberne (gio) | gran/hertz/history (o) | gran/hooke (co) | gran/hooke/history (o) |
| hbond/dreiding/lj (o) | hbond/dreiding/morse (o) | kim | lcbop |
| line/lj (o) | lj/charmm/coul/charmm (cko) | lj/charmm/coul/charmm/implicit (cko) | lj/charmm/coul/long (cgiko) |
| lj/charmm/coul/msm | lj/class2 (cgko) | lj/class2/coul/cut (cko) | lj/class2/coul/long (cgko) |
| lj/cut (cgikot) | lj/cut/coul/cut (cgko) | lj/cut/coul/debye (cgko) | lj/cut/coul/dsf (gko) |
| lj/cut/coul/long (cgikot) | lj/cut/coul/msm (go) | lj/cut/dipole/cut (go) | lj/cut/dipole/long |
| lj/cut/tip4p/cut (o) | lj/cut/tip4p/long (ot) | lj/expand (cgko) | lj/gromacs (cgko) |
| lj/gromacs/coul/gromacs (cko) | lj/long/coul/long (o) | lj/long/dipole/long | lj/long/tip4p/long |
| lj/smooth (co) | lj/smooth/linear (o) | lj96/cut (cgo) | lubricate (o) |
| lubricate/poly (o) | lubricateU | lubricateU/poly | meam (o) |
| mie/cut (o) | morse (cgot) | nb3b/harmonic (o) | nm/cut (o) |
| nm/cut/coul/cut (o) | nm/cut/coul/long (o) | peri/eps | peri/lps (o) |
| peri/pmb (o) | peri/ves | polymorphic | reax |
| rebo (o) | resquared (go) | snap | soft (go) |
| sw (cgkio) | table (gko) | tersoff (cko) | tersoff/mod (ko) |
| tersoff/zbl (ko) | tip4p/cut (o) | tip4p/long (o) | tri/lj (o) |
| yukawa (go) | yukawa/colloid (go) | zbl (o) | |

al pair styles in USER packages, which can be used if LAMMPS is built with the appropriate package.

| | | | |
|---|---|---|---|
| awpmd/cut | coul/cut/soft (o) | coul/diel (o) | coul/long/soft (o) |
| eam/cd (o) | edip (o) | eff/cut | gauss/cut |
| list | lj/charmm/coul/long/soft (o) | lj/cut/coul/cut/soft (o) | lj/cut/coul/long/soft (o) |
| lj/cut/dipole/sf (go) | lj/cut/soft (o) | lj/cut/tip4p/long/soft (o) | lj/sdk (gko) |
| lj/sdk/coul/long (go) | lj/sdk/coul/msm (o) | lj/sf (o) | meam/spline |
| meam/sw/spline | quip | reax/c | sph/heatconduction |
| sph/idealgas | sph/lj | sph/rhosum | sph/taitwater |

# Pair styles

See doc/pair.html for one-line descriptions

- pair_style none - turn off pairwise interactions
- pair_style hybrid - multiple styles of pairwise interactions
- pair_style hybrid/overlay - multiple styles of superposed pairwise interactions

- pair_style adp - angular dependent potential (ADP) of Mishin
- pair_style airebo - AIREBO potential of Stuart
- pair_style beck - Beck potential
- pair_style body - interactions between body particles
- pair_style bop - BOP potential of Pettifor
- pair_style born - Born-Mayer-Huggins potential
- pair_style born/coul/long - Born-Mayer-Huggins with long-range Coulombics
- pair_style born/coul/msm - Born-Mayer-Huggins with long-range MSM Coulombics
- pair_style born/coul/wolf - Born-Mayer-Huggins with Coulombics via Wolf potential
- pair_style brownian - Brownian potential for Fast Lubrication Dynamics
- pair_style brownian/poly - Brownian potential for Fast Lubrication Dynamics with polydispersity
- pair_style buck - Buckingham potential
- pair_style buck/coul/cut - Buckingham with cutoff Coulomb
- pair_style buck/coul/long - Buckingham with long-range Coulombics
- pair_style buck/coul/msm - Buckingham long-range MSM Coulombics
- pair_style buck/long/coul/long - long-range Buckingham with long-range Coulombics
- pair_style colloid - integrated colloidal potential
- pair_style comb - charge-optimized many-body (COMB) potential
- pair_style coul/cut - cutoff Coulombic potential
- pair_style coul/debye - cutoff Coulombic potential with Debye screening
- pair_style coul/dsf - Coulombics via damped shifted forces
- pair_style coul/long - long-range Coulombic potential
- pair_style coul/msm - long-range MSM Coulombics
- pair_style coul/wolf - Coulombics via Wolf potential
- pair_style dipole/cut - point dipoles with cutoff
- pair_style dpd - dissipative particle dynamics (DPD)
- pair_style dpd/tstat - DPD thermostatting
- pair_style dsmc - Direct Simulation Monte Carlo (DSMC)
- pair_style eam - embedded atom method (EAM)
- pair_style eam/alloy - alloy EAM
- pair_style eam/fs - Finnis-Sinclair EAM
- pair_style eim - embedded ion method (EIM)
- pair_style gauss - Gaussian potential
- pair_style gayberne - Gay-Berne ellipsoidal potential
- pair_style gran/hertz/history - granular potential with Hertzian interactions
- pair_style gran/hooke - granular potential with history effects
- pair_style gran/hooke/history - granular potential without history effects

# Relative CPU cost of potentials

See http://lammps.sandia.gov/bench.html#potentials for details
Can estimate how long your simulation will run

| Potential | System | Atoms | Timestep | CPU | LJ Ratio |
|---|---|---|---|---|---|
| Granular | chute flow | 32000 | 0.0001 tau | 5.08e-7 | 0.34x |
| FENE bead/spring | polymer melt | 32000 | 0.012 tau | 5.32e-7 | 0.36x |
| Lennard-Jones | LJ liquid | 32000 | 0.005 tau | 1.48e-6 | 1.0x |
| DPD | pure solvent | 32000 | 0.04 tau | 2.16e-6 | 1.46x |
| EAM | bulk Cu | 32000 | 5 fmsec | 3.59e-6 | 2.4x |
| Tersoff | bulk Si | 32000 | 1 fmsec | 6.01e-6 | 4.1x |
| Stillinger-Weber | bulk Si | 32000 | 1 fmsec | 6.10e-6 | 4.1x |
| EIM | crystalline NaCl | 32000 | 0.5 fmsec | 9.69e-6 | 6.5x |
| SPC/E | liquid water | 36000 | 2 fmsec | 1.43e-5 | 9.7x |
| CHARMM + PPPM | solvated protein | 32000 | 2 fmsec | 2.01e-5 | 13.6x |
| MEAM | bulk Ni | 32000 | 5 fmsec | 2.31e-5 | 15.6x |
| Peridynamics | glass fracture | 32000 | 22.2 nsec | 2.42e-5 | 16.4x |
| Gay-Berne | ellipsoid mixture | 32768 | 0.002 tau | 4.09e-5 | 28.3x |
| AIREBO | polyethylene | 32640 | 0.5 fmsec | 8.09e-5 | 54.7x |
| COMB | crystalline SiO2 | 32400 | 0.2 fmsec | 4.19e-4 | 284x |
| eFF | H plasma | 32000 | 0.001 fmsec | 4.52e-4 | 306x |
| ReaxFF | PETN crystal | 16240 | 0.1 fmsec | 4.99e-4 | 337x |
| ReaxFF/C | PETN crystal | 32480 | 0.1 fmsec | 2.73e-4 | 185x |
| VASP/small | water | 192/512 | 0.3 fmsec | 26.2 | 17.7e6 |
| VASP/medium | CO2 | 192/1024 | 0.8 fmsec | 252 | 170e6 |
| VASP/large | Xe | 432/3456 | 2.0 fmsec | 1344 | 908e6 |

# Bond styles (also angle, dihedral, improper)

- Used for molecules with <span style="color:red">fixed bonds</span>
  - Fix bond/break and bond_style quartic can break them
- To learn what bond styles LAMMPS has ...
  where would you look?

# Bond styles (also angle, dihedral, improper)

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  - Fix bond/break and bond_style quartic can break them
- To learn what bond styles LAMMPS has ...
  where would you look?
- doc/Section_commands.html or doc/bond_style.html

| none | hybrid | class2 | fene |
|------|--------|--------|------|
| fene/expand | harmonic | morse | nonlinear |
| quartic | table | | |

ich can be used if LAMMPS is built with the appropriate package.

| harmonic/shift | harmonic/shift/cut |
|----------------|--------------------|

e used if LAMMPS is built with the appropriate accelerated package.

| class2/omp | fene/omp | fene/expand/omp | harmonic/omp |
|------------|----------|-----------------|--------------|
| harmonic/shift/omp | harmonic/shift/cut/omp | morse/omp | nonlinear/omp |
| quartic/omp | table/omp | | |

- bond_style none - turn off bonded interactions
- bond_style hybrid - define multiple styles of bond interactions

- bond_style class2 - COMPASS (class 2) bond
- bond_style fene - FENE (finite-extensible non-linear elastic) bond
- bond_style fene/expand - FENE bonds with variable size particles
- bond_style harmonic - harmonic bond
- bond_style morse - Morse bond
- bond_style nonlinear - nonlinear bond
- bond_style quartic - breakable quartic bond
- bond_style table - tabulated by bond length

# Long-range Coulombics

KSpace style in LAMMPS lingo, see doc/kspace_style.html

- Options:
  - traditional Ewald, scales as $O(N^{3/2})$
  - PPPM (like PME), scales as $O(N \log(N))$
  - MSM, scales as $O(N)$, lj/cut/coul/msm
- Additional options:
  - non-periodic, PPPM (z) vs MSM (xyz)
  - long-range dispersion (LJ)

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- Additional options:
  - non-periodic, PPPM (z) vs MSM (xyz)
  - long-range dispersion (LJ)
- PPPM is fastest choice for most systems
  - FFTs can scale poorly for large processor counts
- MSM can be faster for low-accuracy or large proc counts
- Pay attention to cutoff & accuracy settings
  - can affect performance dramatically
  - adjust Real vs KSpace work

# Fixes

Most flexible feature in LAMMPS
Allow control of "what" happens "when" within each timestep

Loop over timesteps:

    communicate ghost atoms

    build neighbor list (once in a while)
    compute forces
    communicate ghost forces

    output to screen and files

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Allow control of "what" happens "when" within each timestep

Loop over timesteps:
   fix initial               NVE, NVT, NPT, rigid-body integration
   communicate ghost atoms
   fix neighbor                   insert particles
   build neighbor list (once in a while)
   compute forces
   communicate ghost forces
   fix force          SHAKE, langevin drag, wall, spring, gravity
   fix final          NVE, NVT, NPT, rigid-body integration
   fix end           volume & T rescaling, diagnostics
   output to screen and files

# Fixes

- ∼150 fixes in LAMMPS
- You choose what group of atoms to apply fix to
- Already saw some in obstacle example:
  - fix 1 all nve
  - fix 2 flow temp/rescale 200 1.0 1.0 0.02 1.0
  - fix 3 lower setforce 0.0 0.0 0.0
  - fix 5 upper aveforce 0.0 -0.5 0.0
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- doc/Section_commands.html or doc/fix.html
- If you familiarize yourself with fixes,
  you'll know many things LAMMPS can do
- Many fixes store output accessible by other commands
  - rigid body COM
  - thermostat energy
  - forces before modified

# Computes

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  doc/Section_commands.html or doc/compute.html

| angle/local | atom/molecule | body/local | bond/local | centro/atom | cluster/atom |
|---|---|---|---|---|---|
| cna/atom | com | com/molecule | contact/atom | coord/atom | damage/atom |
| dihedral/local | displace/atom | erotate/asphere | erotate/sphere | erotate/sphere/atom | event/displace |
| group/group | gyration | gyration/molecule | heat/flux | improper/local | inertia/molecule |
| ke | ke/atom | msd | msd/molecule | msd/nongauss | pair |
| pair/local | pe | pe/atom | pressure | property/atom | property/local |
| property/molecule | rdf | reduce | reduce/region | slice | stress/atom |
| temp | temp/asphere | temp/com | temp/deform | temp/partial | temp/profile |
| temp/ramp | temp/region | temp/sphere | ti | voronoi/atom | |

ributed by users, which can be used if LAMMPS is built with the appropriate package.

| ackland/atom | basal/atom | ke/eff | ke/atom/eff | meso_e/atom | meso_rho/atom |
|---|---|---|---|---|---|
| meso_t/atom | temp/eff | temp/deform/eff | temp/region/eff | temp/rotate | |

e styles, which can be used if LAMMPS is built with the appropriate accelerated package.

| pe/cuda | pressure/cuda | temp/cuda | temp/partial/cuda |
|---|---|---|---|

- Key point:
  - computes store their answers
  - other commands invoke them and use the results
  - e.g. thermo output, dumps, fixes
- Output of computes:
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  - extensive vs intensive values

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- Output of computes:
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  - scalar vs vector vs array
  - extensive vs intensive values
- Examples:
  - temp & pressure = global scalar or vector
  - pe/atom = potential energy per atom (vector)
  - displace/atom = displacement per atom (array)
  - pair/local & bond/local = per-neighbor or per-bond info
- Many computes are useful with averaging fixes:
  - fix ave/time, ave/chunk (spatial), ave/atom
  - fix ave/histo, ave/correlate

# Thermo output

One line of output every N timesteps to screen and log file

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- Any scalar can be output:
  - dozens of keywords: temp, pyy, eangle, lz, cpu
  - any output of a compute or fix: c_ID, f_ID[N], c_ID[N][M]
    - fix ave/time stores time-averaged quantities
  - equal-style variable: v_MyVar
  - one value from atom-style variable: v_xx[N]
  - any property for one atom: q, fx, quat, etc

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- Post-process via:
  - tools/python/logplot.py log.lammps X Y (via GnuPlot)
  - tools/python/log2txt.py log.lammps data.txt X Y ...
  - Pizza.py log tool
  - can read thermo output across multiple runs

# Dump output

Snapshot of per-atom values every N timesteps

- See doc/dump.html

# Dump output

Snapshot of per-atom values every N timesteps

- See doc/dump.html
- Styles
  - atom, custom (both native LAMMPS)
    - VMD will auto-read if file named *.lammpstraj
  - xyz for coords only
  - cfg for AtomEye
  - DCD, XTC for CHARMM, NAMD, GROMACS
    - good for back-and-forth runs and analysis
- Two additional styles
  - local: per-neighbor, per-bond, etc info
  - image: instant picture, rendered in parallel

# Dump output

- Any per-atom quantity can be output
  - dozens of keywords: id, type, x, xs, xu, mux, omegax, ...
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  - MPIIO package for parallel dump output
- Post-run conversion
  - tools/python/dump2cfg.py, dump2pdb.py, dump2xyz.py
  - Pizza.py dump, cfg, ensight, pdb, svg, vtk, xyz

# Parallelization in LAMMPS

- Physical domain divided into 3d bricks
- One brick per processor
- Atoms carry properties & topology as they migrate
- Comm of ghost atoms within cutoff
  - 6-way local stencil
- Short-range forces $\Rightarrow$ CPU cost scales as $O(N/P)$

# Parallel performance
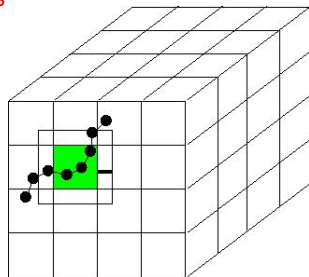
See http://lammps.sandia.gov/bench.html
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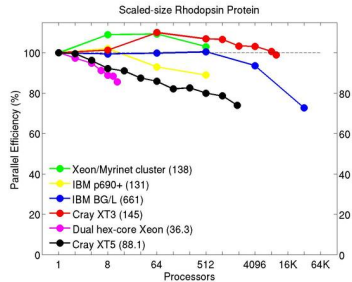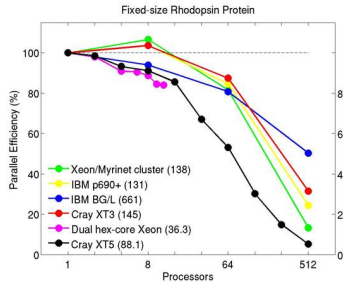
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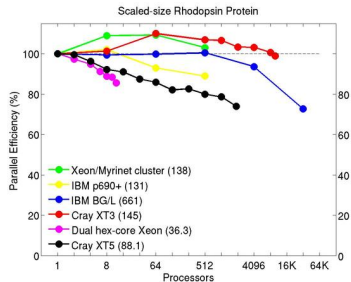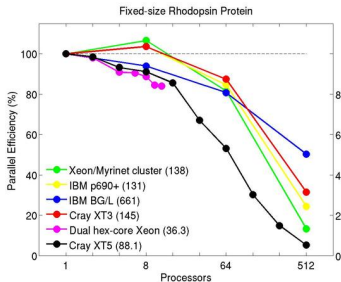


Exercise: run bench/in.lj, change N and P, is it $O(N/P)$ ?
- lmp_linux -v x 2 -v y 2 -v z 2 < in.lj
- mpirun -np 2 lmp_linux < in.lj

# How to speed-up your simulations

See doc/Section_accelerate.html of manual

1. Many ideas for long-range Coulombics
   - PPPM with 2 vs 4 FFTs (smoothed PPPM)
   - PPPM with staggered grid
   - run_style verlet/split
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   - PPPM with 2 vs 4 FFTs (smoothed PPPM)
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   - processor layout
2. GPU, USER-INTEL, USER-OMP, KOKKOS packages
   - GPU for NVIDIA GPUs with multiple cores/GPU
   - USER-INTEL for Intel CPU optimization and Xeon Phi
   - USER-OMP for OpenMP on multicore nodes
   - KOKKOS for GPUs, OpenMP, and Xeon Phi
     - see Kokkos talk by Stan Moore on Thurs AM
   - Benchmark data at http://lammps.sandia.gov/bench.html

# How to speed-up your simulations

3. **Increase time scale** via timestep size
   - fix shake for rigid bonds (2 fs)
   - run_style respa for hierarchical timesteps (4 fs)

4. **Increase length scale** via coarse graining
   - all-atom vs united-atom vs bead-spring
   - mesoscale models:
     - ASPHERE, BODY, COLLOID, FLD packages
     - GRANULAR, PERI, RIGID, SRD packages
     - see doc/Section_packages.html for details

# Quick tour of more advanced topics

- Units
  - see doc/units.html
  - LJ, real, metal, cgs, si
  - all input/output in one unit system
- Ensembles
  - see doc/Section_howto.html 6.16
  - one or more thermostats (by group)
  - single barostat
  - rigid body dynamics
- Hybrid models
  - pair_style hybrid and hybrid/overlay
  - atom_style hybrid sphere bond ...

# Quick tour of more advanced topics

- **Aspherical particles**
  - see doc/Section_howto.html 6.14
  - ellipsoidal, lines, triangles, rigid bodies
  - ASPHERE package
- **Mesoscale and continuum models**
  - COLLOID, FLD, SRD packages for NPs and colloids
  - PERI package for Peridynamics
  - USER-ATC package for atom-to-continuum (FE)
  - USER-SPH, USER-SMD packages for smoothed particle hydro
  - GRANULAR package for granular media
  - add-on LIGGGHTS package for DEM
    - www.liggghts.com/www.cfdem.com
    - see talk by Christoph Kloss on Fri AM
  - breakout session B1 on Thurs

# Quick tour of more advanced topics

- Multi-replica modeling
  - see doc/Section_howto.html 6.14
  - parallel tempering
  - PRD, TAD, NEB
- Load balancing
  - balance command for static LB
  - fix balance command for dynamic LB
  - adjusting proc dividers, or recursive coordinate bisection
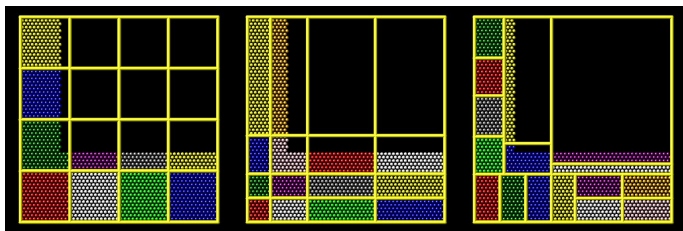
# Quick tour of more advanced topics

- Energy minimization
  - Via usual dynamics
    - pair_style soft
    - fix nve/limit and fix viscous
  - Via gradient-based minimization
    - min_style cg, htfn, sd
  - Via damped-dynamics minimization
    - min_style quickmin and fire
    - used for nudged-elastic band (NEB)

# Quick tour of more advanced topics

Use LAMMPS as a library

- doc/Section_howto.html 6.10 and 6.19
- C-style interface (C, C++, Fortran, Python)
- examples/COUPLE dir
- python and python/examples directories

# What have people done with LAMMPS?

- Pictures: http://lammps.sandia.gov/pictures.html
- Movies: http://lammps.sandia.gov/movies.html

| | | | |
|---|---|---|---|
| | evaporation self-assembly | | Compression of nanoparticles |
| | GCMC model of zeolite occupancy | | self-assembling nanofibers from Thiophene-peptide oligomers |
| | layer-by-layer self assembly | | smoothed particle hydrodynamics (SPH) models |
| | dislocations moving thru grain boundaries | | electron force field for non-adiabatic dynamics |
| | granular particles flowing from hopper | | granular Discrete Element Method (DEM) models |
| | fiber dynamics | | brazing of two-metal system |
| | Peridynamics mesoscale modeling of impact fracture | | shear faults in a model brittle solid |
| | stick/slip and polymer flow on rough surfaces | | crystallization of polyethylene melt |
| | melting of polycrystalline metal | | deformation and void nucleation under shock loading |
| | dynamics of an isolated edge dislocation | | cavitation in liquid metal |
| | nanoprecipitates and shock induced plasticity | | Brazil nut effect |
| | ultra-thin Cu nanowire formation | | Cu nanowire loading and unloading |
| | Au nanowire formation and extension | | flow of water and ions thru a silica pore |
| | metal response to He bubble formation | | dynamics of rhodopsin protein in lipid membrane |
| | CO2 escaping from binding pocket of RuBisCO protein | | C-terminus of RuBisCO closing over binding pocket |
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  - authors, titles, abstracts for 1000s of papers

# Customizing and modifying LAMMPS

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- Resources:
    - doc/Section_modify.html
    - doc/PDF/Developer.pdf
        - class hierarchy & timestep structure
    - Links on LAMMPS web site:
        - slides for hackers/developers breakout of past workshops
        - ditto for slides on Tutorials link of web page
- Come to developers breakout session A3 on Thurs
- Please contribute your new code to the LAMMPS distro!
    - doc/Section modify 15:
        Submitting new features for inclusion in LAMMPS