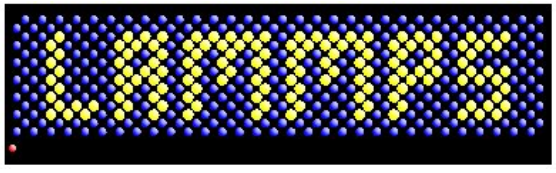
Lecture #3 – Styles, styles, styles

Steve Plimpton
Sandia National Labs
sjplimp@sandia.gov

7th LAMMPS Workshop Tutorial
Virtual meeting – August 2021



Center for Computing Research

Sandia National Laboratories

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

National Nuclear Security Administration

Goals for this lecture

Teach you ...

- What styles are in LAMMPS
- The most versatile styles and what they do
- How styles let you tailor your LAMMPS simulation

What is a style in LAMMPS lingo

- A command with many variants
  - pair_style ⇒ pair_style lj/cut, pair_style eam, etc
  - fix ⇒ fix nve, fix rigid/small, etc
- Why not command names = pair or fix_style ?
  - single instance: command name includes style
  - many instances: command name w/out style
- A virtual parent class with many derived child classes
  - parent = src/pair.cpp or src/fix.cpp
  - children = pair_lj_cut.cpp, pair_eam.cpp, etc
  - children = fix_nve.cpp, fix_rigid_small.cpp, etc

20 different styles in current LAMMPS

Most are invoked as input script commands, some are internal

atom	25	sets of per-atom properties
pair	230	pairwise and manybody potentials
bond/angle/dihedral	15/20/15	intra-molecular interactions
kspace	15	long-range Coulombic solvers
fix	225	operations while timestepping
compute	140	diagnostic calculations
region	8	geometric regions
dump	25	output of simulation snapshots
integrate	2	Verlet or rRESPA algorithms
minimize	9	energy minimization algorithms
command	45	added input script commands
		create_box, create_atoms, run, etc

Pair styles

- LAMMPS lingo for interatomic potentials or force fields
- Define how atoms interact each other
  - short-range portion only
- Critical choice to make for your model and material
- Trade-offs in accuracy vs computational cost
- A pair style can be pair-wise or many-body
  - LJ, Coulombic, Buckingham, Morse, Yukawa, ...
  - EAM, Tersoff, REBO, ReaxFF, ...
- Short-range Coulombics included in pair style
  - lj/cut, lj/cut/coul/cut, lj/cut/coul/long, lj/cut/coul/wolf
  - done to optimize inner loop

Categories of pair styles for different materials

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

Categories of pair styles for different materials

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

- Pair table for tabulation of any pair-wise interaction
- Pair hybrid enables modeling of hybrid systems
  - polymers on metal
  - CNTs in water
  - solid-solid interface between 2 materials

List of pair styles available natively in LAMMPS

See website Commands ⇒ Pair Styles
Annotated with (gikot) for 5 accelerated variants

5.8. Pair_style potentials

All LAMMPS pair_style commands. Some styles have accelerated versions. This is indicated by additional letters in parenthesis: g = GPU, i = INTEL, k = KOKKOS, o = OPENMP, t = OPT.

none	zero	hybrid (k)	hybrid/overlay (k)
hybrid/scaled	kim	list	
adp (o)	agni (o)	airebo (io)	airebo/morse (io)
atm	awpmd/cut	beck (go)	body/nparticle
body/rounded/polygon	body/rounded/polyhedron	bop	born (go)
born/coul/dsf	born/coul/dsf/cs	born/coul/long (go)	born/coul/long/cs (g)

- LAMMPS pair kim = interface to OpenKIM repository
- Ellad Tadmor talk: Thu early session
- OpenKIM breakout: Fri

One-line descriptions of pair styles

See pair_style doc page

- none - turn off pairwise interactions
- hybrid - multiple styles of pairwise interactions
- hybrid/overlay - multiple styles of superposed pairwise interactions
- hybrid/scaled - multiple styles of scaled superposed pairwise interactions
- zero - neighbor list but no interactions
- adp - angular dependent potential (ADP) of Mishin
- agni - AGNI machine-learning potential
- airebo - AIREBO potential of Stuart
- airebo/morse - AIREBO with Morse instead of LJ
- atm - Axilrod-Teller-Muto potential
- awpmd/cut - Antisymmetrized Wave Packet MD potential for atoms and electrons
- beck - Beck potential
- body/nparticle - interactions between body particles
- body/rounded/polygon - granular-style 2d polygon potential
- body/rounded/polyhedron - granular-style 3d polyhedron potential
- bop - BOP potential of Pettifor

Relative CPU cost of different potentials is dramatic

See website Benchmark ⇒ Interatomic potential for details
Useful to estimate how long your simulation will run

Potential	System	# Atoms	Timestep	Neighs/atom	Memory	CPU	LJ Ratio	F
Granular	chute flow	32000	0.0001 tau	7.2	33 Mb	2.08e-7	0.26x	
FENE bead/spring	polymer melt	32000	0.012 tau	9.7	8.4 Mb	2.86e-7	0.36x	
Lennard-Jones	LJ liquid	32000	0.005 tau	76.9	12 Mb	8.01e-7	1.0x	
DPD	pure solvent	32000	0.04 tau	41.3	9.4 Mb	1.22e-6	1.53x	
EAM	bulk Cu	32000	5 fmsec	75.5	13 Mb	1.87e-6	2.34x	
REBO	polyethylene	32640	0.5 fmsec	149	33 Mb	3.18e-6	3.97x	
Stillinger-Weber	bulk Si	32000	1 fmsec	30.0	11 Mb	3.28e-6	4.10x	
Tersoff	bulk Si	32000	1 fmsec	16.6	9.2 Mb	3.74e-6	4.67x	
AIREBO	polyethylene	32640	0.5 fmsec	681	101 Mb	3.25e-5	40.6x	
ReaxFF/C	PETN crystal	32480	0.1 fmsec	667	976 Mb	1.09e-4	136x	
COMB	crystalline SiO2	32400	0.2 fmsec	572	85 Mb	2.00e-4	250x	
eFF	H plasma	32000	0.001 fmsec	5066	365 Mb	2.16e-4	270x	
ReaxFF	PETN crystal	16240	0.1 fmsec	667	425 Mb	2.84e-4	354x	

Bond styles (also angle, dihedral, improper)

LAMMPS lingo for intra-molecular 2,3,4-body interactions

- Used for molecules with fixed covalent bonds
  - fix bond/react command can form and break them
  - Jake Gisssinger talk: Thu late session
- To learn what bond styles LAMMPS has ... where to look?

Bond styles (also angle, dihedral, improper)

LAMMPS lingo for intra-molecular 2,3,4-body interactions

- Used for molecules with fixed covalent bonds
  - fix bond/react command can form and break them
  - Jake Gisssinger talk: Thu late session
- To learn what bond styles LAMMPS has ... where to look?
- Website Commands ⇒ Bond Styles or
  bond_style doc page

5.9. Bond_style potentials

All LAMMPS bond_style commands. Some styles have accelerated versions. This is indicated by additional letters in parenthesis: g = GPU, i = INTEL, k = KOKKOS, o = OPENMP, t = OPT.

none	zero	hybrid	
class2 (ko)	fene (iko)	fene/expand (o)	gaussian
gromos (o)	harmonic (iko)	harmonic/shift (o)	harmonic/shift/cut (o)
mm3	morse (o)	nonlinear (o)	oxdna/fene
oxdna2/fene	oxrna2/fene	quartic (o)	special
table (o)			

- none - turn off bonded interactions
- zero - topology but no interactions
- hybrid - define multiple styles of bond interactions
- class2 - COMPASS (class 2) bond
- fene - FENE (finite-extensible non-linear elastic) bond
- fene/expand - FENE bonds with variable size particles
- gaussian - multicentered Gaussian-based bond potential
- gromos - GROMOS force field bond
- harmonic - harmonic bond
- harmonic/shift - shifted harmonic bond

KSpace styles

LAMMPS lingo for long-range Coulombic solvers
Web Commands ⇒ Kspace Styles or kspace_style doc page

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

KSpace styles

LAMMPS lingo for long-range Coulombic solvers
Web Commands ⇒ Kspace Styles or kspace_style doc page

- Options:
  - traditional Ewald, scales as $O(N^{3/2})$
  - PPPM (like PME), scales as $O(N \log(N))$
  - MSM, scales as $O(N)$
- Additional options:
  - non-periodic: PPPM (z) or MSM (xyz)
  - long-range dispersion (LJ) or dipolar
- 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
  - adjusts Real-space versus KSpace work
  - can affect performance (see logfile timings)

Fix styles

Most flexible feature in LAMMPS
Fixes enable control of what happens when in a timestep
Internal flags determine when different methods of fix are invoked

communicate ghost coords

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

output to screen and files

Fix styles

Most flexible feature in LAMMPS
Fixes enable control of what happens when in a timestep
Internal flags determine when different methods of fix are invoked

Loop over timesteps:

fix initial	NVE, NVT, NPT, rigid-body integration
communicate ghost coords	
fix neighbor	insert/delete 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	

More on fix styles

- Assign each fix a unique alphanumeric ID
- Choose what group of atoms to apply fix to

More on fix styles

- Assign each fix a unique alphanumeric ID
- Choose what group of atoms to apply fix to
- Examples of groups in.obstacle script:
  - fix 1 all nve
  - fix 2 flow temp/rescale 200 1.0 1.0 0.02 1.0
  - fix 5 upper aveforce 0.0 -0.5 0.0
  - fix 6 flow addforce 1.0 0.0 0.0

More on fix styles

- Assign each fix a unique alphanumeric ID
- Choose what group of atoms to apply fix to
- Examples of groups in.obstacle script:
  - fix 1 all nve
  - fix 2 flow temp/rescale 200 1.0 1.0 0.02 1.0
  - fix 5 upper aveforce 0.0 -0.5 0.0
  - fix 6 flow addforce 1.0 0.0 0.0
- An input script may use dozens of fixes
  - same fix multiple times, on different groups of atoms
- Fixes can store output or persistent info
  - thermostat energy, forces on wall, time-zero atom coords
  - accessible by other commands or variables or log/dump output

More on fix styles

- Assign each fix a unique alphanumeric ID
- Choose what group of atoms to apply fix to
- Examples of groups in.obstacle script:
  - fix 1 all nve
  - fix 2 flow temp/rescale 200 1.0 1.0 0.02 1.0
  - fix 5 upper aveforce 0.0 -0.5 0.0
  - fix 6 flow addforce 1.0 0.0 0.0
- An input script may use dozens of fixes
  - same fix multiple times, on different groups of atoms
- Fixes can store output or persistent info
  - thermostat energy, forces on wall, time-zero atom coords
  - accessible by other commands or variables or log/dump output

If familiarize yourself with fixes,

you'll know many, many things LAMMPS can do

Website Commands $\Rightarrow$ Fix Styles or fix doc page

Compute styles

LAMMPS lingo for a diagnostic calculation

- Calculate some property of the system
- Always for the current timestep
- Defining a compute in an input script does not invoke it
- Fixes or output commands (thermo, dump) invoke computes, only on timesteps when needed

Compute styles

LAMMPS lingo for a diagnostic calculation

- Calculate some property of the system
- Always for the current timestep
- Defining a compute in an input script does not invoke it
- Fixes or output commands (thermo, dump) invoke computes, only on timesteps when needed

Examples:

- Thermostat fixes: compute temp, temp/asphere
- Time averaging fixes:
  fix ave/time, ave/chunk (spatial), ave/atom, ave/histo
- Thermo output to logfile: compute temp, pe, press
- Dump files: compute coord/atom, cna/atom, voronoi/atom

More on compute styles

- All computes store output:
  - global vs per-atom vs local info
    - computes with /atom suffix produce per-atom info
    - computes with /local suffix produce local info
  - scalar vs vector vs array data structure
  - accessible by other commands or variables or log/dump output
- 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

More on compute styles

- All computes store output:
  - global vs per-atom vs local info
    - computes with /atom suffix produce per-atom info
    - computes with /local suffix produce local info
  - scalar vs vector vs array data structure
  - accessible by other commands or variables or log/dump output
- 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

To learn what compute styles LAMMPS has ...
Website Commands ⇒ Compute Styles or compute doc page