Styles, styles, styles

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Virtual meeting – August 2023

Goals for this lecture

Teach you ...

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

Motivation: If you familiarize yourself with styles,
you'll know many, many things LAMMPS can do

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
Asterisk means only a single instance of that style (at a time)

atom*	27	sets of per-atom properties
pair*	275	pairwise/manybody potentials
bond*/angle*/dihedral*	25/20/15	intra-molecular interactions
kspace*	20	long-range Coulombic solvers
fix	250	operations while timestepping
compute	160	diagnostic calculations
region	8	geometric regions
dump	25	output of simulation snapshots
integrate*	2	Verlet or rRESPA algorithms
minimize*	9	energy minimization algorithms
command	50	added input script commands: create_box, create_atoms, run

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
  - two talks later today on this topic
  - literature search can also be helpful
- 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

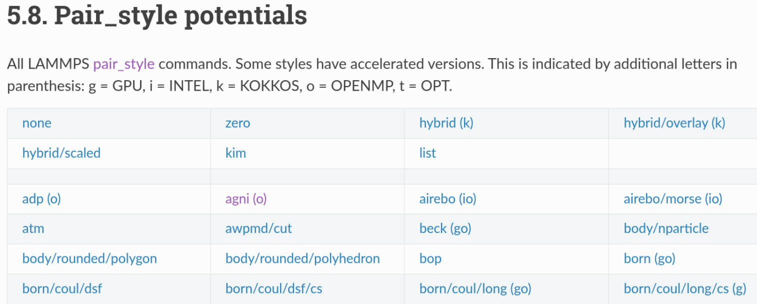
Categories of pair styles for different materials

- 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

- 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 different materials

List of pair styles available natively in LAMMPS

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



5.8. Pair_style potentials

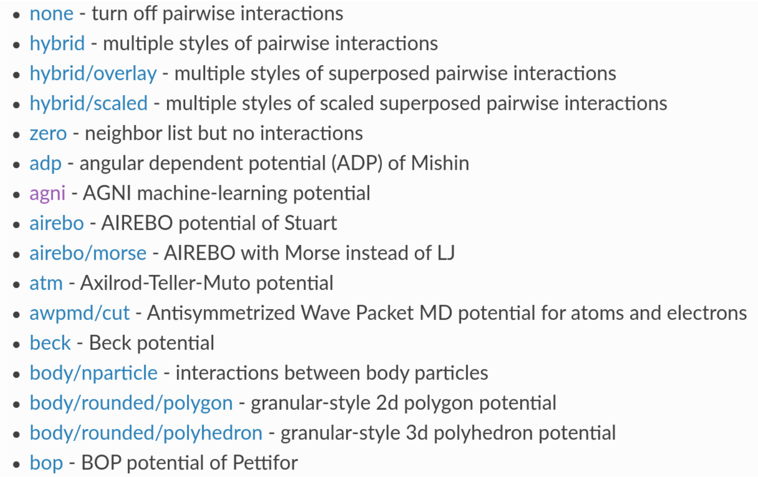
All LAMMPS pair_style commands. Some styles have accelerated versions. This is indicated by additional letters in parenthesis: g = GPU, i = INTEL, k = KOKKOS, o = OPENMP, t = OPT.

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)

- pair kim command = interface to OpenKIM repository
- 2 talks: today and Ellad Tadmor talk: Wed early session
- OpenKIM breakout: Fri

One-line descriptions of pair styles

See pair_style doc page

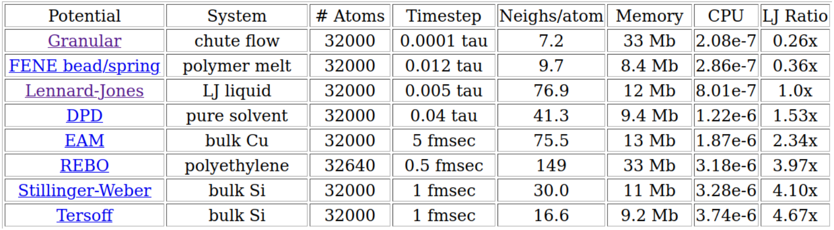


- none - turn off pairwise interactions
- hybrid - multiple styles of pairwise interactions
- hybrid/overlay - multiple styles of superposed pairwise interactions
- hybrid/scaled - multiple styles of scaled superposed pairwise interactions
- zero - neighbor list but no interactions
- adp - angular dependent 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

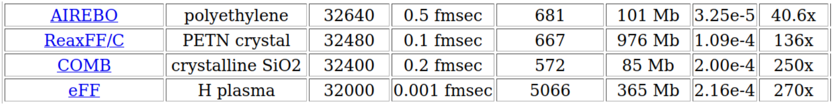
Relative CPU cost of different potentials is dramatic

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
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

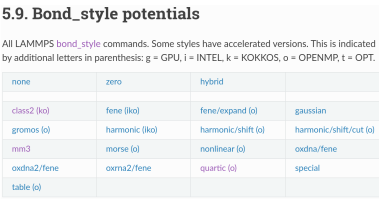


AIREBO	polyethylene	32640	0.5 fmsec	681	101 Mb	3.25e-5	40.6x
ReaxFF/C	PETN crystal	32480	0.1 fmsec	667	976 Mb	1.09e-4	136x
COMB	crystalline SiO2	32400	0.2 fmsec	572	85 Mb	2.00e-4	250x
eFF	H plasma	32000	0.001 fmsec	5066	365 Mb	2.16e-4	270x

Bond styles (also angle, dihedral, improper)

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

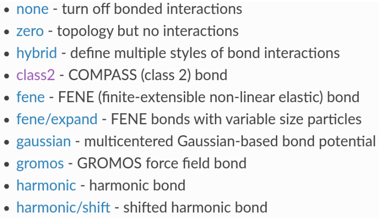
- Used for molecules with fixed covalent bonds
  - fix bond/react command can form and break them
- To learn what bond styles LAMMPS has ... where to look?
- Website Commands ⇒ Bond Styles or
  bond_style doc page



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
Website Commands ⇒ Kspace Styles or kspace_style doc page

- Methods:
  - 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
  - cutoff adjusts Real-space versus K-Space 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 a fix are invoked

MD Loop over timesteps:

```
  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 a fix are invoked

MD 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 & temp 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
- Examples of groups in 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 different fixes
  - or same fix multiple times, on different groups of atoms
- Fixes can produce output or store persistent per-atom info
  - thermostat energy, forces on wall, time-zero atom coords
  - accessible by other commands or variables or log/dump output

Website Commands ⇒ Fix Styles or fix doc page

Compute styles

LAMMPS lingo for a diagnostic computation

- 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) can take computes as input, invoke only on timesteps when needed

Examples:

- Thermostat fixes: compute temp, temp/asphere
- Time averaging fixes operating on computes: 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 (per-atom vector)
  - displace/atom = displacement per atom (per-atom array)
  - pair/local & bond/local = local per-neighbor or per-bond info

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