CHAPTER

NINE

EXAMPLE SCRIPTS

The LAMMPS distribution includes an examples subdirectory with many sample problems. Many are 2d models that run quickly and are straightforward to visualize, requiring at most a couple of minutes to run on a desktop machine. Each problem has an input script (in.*) and produces a log file (log.*) when it runs. Some use a data file (data.*) of initial coordinates as additional input. A few sample log file run on different machines and different numbers of processors are included in the directories to compare your answers to. E.g. a log file like log.date.crack.foo.P means the "crack" example was run on P processors of machine "foo" on that date (i.e. with that version of LAMMPS).

Many of the input files have commented-out lines for creating dump files and image files.

If you uncomment the *dump* command in the input script, a text dump file will be produced, which can be animated by various visualization programs.

If you uncomment the *dump image* command in the input script, and assuming you have built LAMMPS with a JPG library, JPG snapshot images will be produced when the simulation runs. They can be quickly post-processed into a movie using commands described on the *dump image* doc page.

Animations of many of the examples can be viewed on the Movies section of the LAMMPS website.

There are two kinds of subdirectories in the examples folder. Lower case named directories contain one or a few simple, quick-to-run problems. Upper case named directories contain up to several complex scripts that illustrate a particular kind of simulation method or model. Some of these run for longer times, e.g. to measure a particular quantity.

Lists of both kinds of directories are given below.

9.1 Lowercase directories

accelerate	run with various acceleration options (OpenMP, GPU, Phi)
airebo	polyethylene with AIREBO potential
atm	Axilrod-Teller-Muto potential example
balance	dynamic load balancing, 2d system
body	body particles, 2d system
bpm	BPM simulations of pouring elastic grains and plate impact
cmap	CMAP 5-body contributions to CHARMM force field
colloid	big colloid particles in a small particle solvent, 2d system
comb	models using the COMB potential
controller	use of fix controller as a thermostat
coreshell	core/shell model using CORESHELL package
crack	crack propagation in a 2d solid
deposit	deposit atoms and molecules on a surface

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dipole	point dipolar particles, 2d system
dreiding	methanol via Dreiding FF
eim	NaCl using the EIM potential
ellipse	ellipsoidal particles in spherical solvent, 2d system
flow	Couette and Poiseuille flow in a 2d channel
friction	frictional contact of spherical asperities between 2d surfaces
mc	Monte Carlo features via fix gcmc, widom and other commands
granregion	use of fix wall/region/gran as boundary on granular particles
hugoniostat	Hugoniostat shock dynamics
hyper	global and local hyperdynamics of diffusion on Pt surface
indent	spherical indenter into a 2d solid
kim	use of potentials from the OpenKIM Repository
mdi	use of the MDI package and MolSSI MDI code coupling library
meam	MEAM test for SiC and shear (same as shear examples)
melt	rapid melt of 3d LJ system
micelle	self-assembly of small lipid-like molecules into 2d bilayers
min	energy minimization of 2d LJ melt
msst	MSST shock dynamics
multi	multi neighboring for systems with large interaction disparities
nb3b	use of non-bonded 3-body harmonic pair style
neb	nudged elastic band (NEB) calculation for barrier finding
nemd	non-equilibrium MD of 2d sheared system
obstacle	flow around two voids in a 2d channel
peptide	dynamics of a small solvated peptide chain (5-mer)
peri	Peridynamic model of cylinder impacted by indenter
pour	pouring of granular particles into a 3d box, then chute flow
prd	parallel replica dynamics of vacancy diffusion in bulk Si
python	using embedded Python in a LAMMPS input script
qeq	use of the QEQ package for charge equilibration
rdf-adf	computing radial and angle distribution functions for water
reax	RDX and TATB models using the ReaxFF
rerun	use of rerun and read_dump commands
rheo	RHEO simulations of fluid flows and phase transitions
rigid	rigid bodies modeled as independent or coupled
shear	sideways shear applied to 2d solid, with and without a void
snap	NVE dynamics for BCC tantalum crystal using SNAP potential
srd	stochastic rotation dynamics (SRD) particles as solvent
streitz	use of Streitz/Mintmire potential with charge equilibration
tad	temperature-accelerated dynamics of vacancy diffusion in bulk Si
threebody	regression test input for a variety of manybody potentials
tracker	track interactions in LJ melt
vashishta	use of the Vashishta potential
voronoi	Voronoi tesselation via compute voronoi/atom command

Here is how you can run and visualize one of the sample problems:

```
cd indent
cp ../../src/lmp_linux .          # copy LAMMPS executable to this dir
lmp_linux -in in.indent           # run the problem
```

Running the simulation produces the files *dump.indent* and *log.lammps*. You can visualize the dump file of snapshots with a variety of third-party tools highlighted on the Visualization page of the LAMMPS website.

If you uncomment the *dump image* line(s) in the input script a series of JPG images will be produced by the run (assuming you built LAMMPS with JPG support; see the *Build_settings* page for details). These can be viewed individually or turned into a movie or animated by tools like ImageMagick or QuickTime or various Windows-based tools. See the *dump image* page for more details. E.g. this Imagemagick command would create a GIF file suitable for viewing in a browser.

```
% convert -loop 1 *.jpg foo.gif
```

9.2 Uppercase directories

ASPHERE	various aspherical particle models, using ellipsoids, rigid bodies, line/triangle particles, etc
COUPLE	examples of how to use LAMMPS as a library
DIFFUSE	compute diffusion coefficients via several methods
ELASTIC	compute elastic constants at zero temperature
ELASTIC_T	compute elastic constants at finite temperature
HEAT	compute thermal conductivity for LJ and water via fix ehex
KAPPA	compute thermal conductivity via several methods
MC-LOOP	using LAMMPS in a Monte Carlo mode to relax the energy of a system in a input script loop
PACKAGES	examples for specific packages and contributed commands
SPIN	examples for features of the SPIN package
UNITS	examples that run the same simulation in lj, real, metal units
VISCOSITY	compute viscosity via several methods

Nearly all of these directories have README files which give more details on how to understand and use their contents.

The PACKAGES directory has a large number of subdirectories which correspond by name to specific packages. They contain scripts that illustrate how to use the command(s) provided in those packages. Many of the subdirectories have their own README files which give further instructions. See the *Packages_details* doc page for more info on specific packages.