**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](https://www.lammps.org/viz.html).

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](https://www.lammps.org/movies.html).

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.

# 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 |

continues on next page

**401**

**LAMMPS Documentation, Release 29Aug2024**

Table 1 – continued from previous page

|  |  |
| --- | --- |
| 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](https://openkim.org/) |
| 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 . lmp\_linux -in in.indent

# copy LAMMPS executable to this dir # 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](https://www.lammps.org/viz.html) page of the LAMMPS website.

**402 Chapter 9. Example scripts**

**LAMMPS Documentation, Release 29Aug2024**

If you uncomment the *dump image* line(s) in the input script a series of JPG images will be produced by the run (assum- ing 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

# 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.

**9.2. Uppercase directories** **403**