

What is LAMMPS

LAMMPS is a freely available (GPL) classical molecular dynamics code, and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator. LAMMPS has potentials for solid-state materials (metals, semiconductors) and soft matter (biomolecules, polymers) and coarse-grained or mesoscopic systems. It can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale. LAMMPS runs on single processors or in parallel using message-passing techniques and a spatial-decomposition of the simulation domain. The code is designed to be easy to modify or extend with new functionality. It is distributed by Sandia National Laboratories, a US Department of Energy laboratory.

LAMMPS Functionality

LAMMPS includes the following features and functionality:

- Running in parallel using MPI or OpenMP
- Various particle and model types (atoms, coarse-grained particles, united-atom polymers or organic molecules, all-atom polymers, organic molecules, proteins, DNA, metals, granular materials, coarse-grained mesoscale models, and many more)
- Various types of force fields (pairwise potentials, charged pairwise potentials, manybody potentials, charge equilibration, electron force field, coarse-grained potentials, mesoscopic potentials, bond potentials, angle potentials, dihedral potentials, improper potentials, and many more)
- Atom creation (read in atom coordinates from files, create atoms on one or more lattices, delete geometric or logical groups of atoms, replicate existing atoms multiple times, displace atoms)
- Ensembles, constraints and boundary conditions (2D or 3D systems, orthogonal or non-orthogonal, simulation domains, constant NVE, NVT, NPT, NPH, Parinello/Rahman integrators, thermostatting options for groups and geometric regions of atoms, pressure control via Nose/Hoover or Berendsen barostatting in 1 to 3 dimensions, simulation box deformation, harmonic (umbrella) constraint forces, and many more)
- Integrators (velocity-Verlet integrator, Brownian dynamics, rigid body integration, energy minimization via conjugate gradient or steepest descent relaxation, rRESPA hierarchical timestepping, rerun command for post-processing of dump files)
- Diagnostics, multi-replica models, real-time visualisation, dynamic load balancing and many more

Step 1 - Log in

The example used in this guide is configured to run on the Swansea Sandy Bridge cluster. Connect to `login.hpcwales.co.uk` with your HPC Wales user credentials using your preferred method (e.g. PuTTY from a Windows machine or ssh from any Linux terminal), then

`ssh sw-sb-log-001` to connect to the Swansea system.

The steps below involve typing commands (**in bold font**) in the terminal window.

Step 2 - Load a LAMMPS module

A number of LAMMPS binary packages are available.

- List pre-installed LAMMPS versions:
`module avail lammmps`
- Load the default LAMMPS module (Intel build, MPI):
`module load lammmps`
- Confirm the loaded modules. All dependencies are handled automatically via the module file:
`module list`

Step 3 - Create a directory

From your home directory, create a directory to hold LAMMPS user files:

```
cd ~  
mkdir lammmps
```

Step 4 - Obtain a test case

Two test cases are provided with the installation at

```
/app/chemistry/lammmps/27Oct11/sb/intel-13.0/intel-4.1/example
```

Copy the input file and job scripts one of the examples to your user space:

```
cd lammmps  
cp /app/chemistry/lammmps/27Oct11/sb/intel-13.0/intel-4.1/example/in.melt .  
cp /app/chemistry/lammmps/27Oct11/sb/intel-13.0/intel-4.1/example/lampsexample1.SLURM.q .
```

Step 5 - Submit a job

Now you are ready to run the example with the supplied job scripts.

- From your working directory, submit the job by: `sbatch lampsexample1.SLURM.q`
- Check the job queue by: `squeue`
- When the job finishes, it will have created an output file called `LammmpsEx1.o.<JobID>` where `<JobID>` is the ID generated by the system.
- Compare your job output with the reference output file

```
/app/chemistry/lammmps/27Oct11/sb/intel-13.0/intel-4.1/example/LammmpsEx1.o
```

References

Documentation and source code is available at the LAMMPS website:

<http://lammps.sandia.gov/>

A variety of useful tutorials are also available at: <http://lammps.sandia.gov/tutorials>