LAMMPS

Purpose: Molecular Dynamics
Latest version: 23Jun2022
License: Free of use
GNU GPL _ext-link
Website: *http://lammps.sandia.gov/ _ext-link*

LAMMPS is a classical molecular dynamics application.

It performs atomistic or coarse-grained simulations of molecular, macromolecular and mesoscale systems with a variety of force fields.

SLURM Submit script example

More information about the submit script can be found using the ***Job Script Generator***.

lammps_example.slm

```
#!/bin/bash
#SBATCH -J lammps_example
#SBATCH -e lammps_example.err
#SBATCH -o lammps_example.out
#SBATCH -p std
#SBATCH -n 1
#SBATCH -t 0-02:00

module load apps/lammps/31Aug2018

##
#  Modify the input and output files!
INPUT_FILE=lammps_example.in
OUTPUT_FILE=lammps_example.log

cp -r ${SLURM_SUBMIT_DIR}/${INPUT_FILE}
${SCRATCH}
cd ${SCRATCH}

srun lmp_mpi -in ${INPUT_FILE} > ${OUTPUT_FILE}

cp ./${OUTPUT_FILE} ${SLURM_SUBMIT_DIR}
```

Sbatch options:

The options shown in the example are detailed below. For more information and a more comprehensive list of available options, see the ***sbatch command page***.

- **-J**: Name for the job's allocation.
- **-e**: Name of the sterr redirection filename.
- **-o**: Name of the stdout redirection filename.
- **-p**: Name of the partition (queue) where the job will be submited.
- **-n**: Number of tasks.
- **-c**: Number of cores per task.
- **-t**: Set the job's time limit. If the job don't finish before the time runs out, it will be killed.