LAMMPS

LAMMPS is a highly parallized Molecular Dynamics Simulator which uses MPI and OpenMP on CPUs or CUDA to run on GPUs.

Short-Info

LAMMPS	
Category	MD-Simulations
Usage	CPU or GPU
Module-Versions	
LAMMPS/stable_12Dec2018	

Examples

On CPU with MPI

```
#PBS -l select=4:ncpus=1:mpiprocs=1:mem=5G
inputFile="in.melt"

module load LAMMPS/stable_12Dec2018

cd $PBS_O_WORKDIR

MPICPUS=$(cat $PBS_NODEFILE | wc -l)

mpirun -n $MPICPUS lmp -in $inputFile > in.melt.output
```

On GPU

```
#PBS -l select=1:ncpus=1:mem=5G:ngpus=1
inputFile="in.melt"

module load LAMMPS/stable_12Dec2018

cd $PBS_O_WORKDIR

lmp -sf gpu -in $inputFile > in.melt.output
```