Using LAMMPS on HPC clusters:

What is LAMMPS?

LAMMPS also stands for Large-scale Atomic/Molecular Massively Parallel Simulator. It is a classical molecular dynamics simulation code with a focus in materials modelling, running smoothly on parallel computers. It is an open-source code distributed under GNU Public License.

The documentation for the LAMMPS is found on:

https://docs.lammps.org/Manual.html

Versions Available:

physical/LAMMPS/gcc/110917

physical/LAMMPS/gcc/220918-gpu

physical/LAMMPS/intel/171116-avx

physical/LAMMPS/gcc/22Aug2018

physical/LAMMPS/intel/03Mar2020

physical/LAMMPS/gcc/050218

physical/LAMMPS/intel/Oct292020

physical/LAMMPS/intel/220918-gpu

physical/LAMMPS/gcc/220918

physical/LAMMPS/intel/110917

physical/LAMMPS/gcc/160416

physical/LAMMPS/intel/220918

How to load a version of LAMMPS?

To load a version of LAMMPS on the HPC on current terminal session, use the following command:

module avail physical/LAMMPS≠

You will see many versions listed. Select one which fits your project. For this example, I am loading:

module load physical/LAMMPS/gcc/22Aug2018a.

Verify by using this command:

module list

How to use LAMMPS on the cluster?

Here is one example of how to use the LAMMPS on the cluster. Example simulations are in: /share/apps/lammps/lammps/examples.

```
mkdir ~/lammpstest       # Make a directory on home
cd /share/apps/lammps/lammps/examples/flow        #Go to example files


cp * ~/lammpstest                #Copy everything into lammpstest folder
```

Now, after copying an example simulation, we need to make a script to run the example.

The Script:

```
#!/bin/bash
$SBATCH -J Jobname # Jobname
#SBATCH -n 8       # Task per node
#SBATCH -C intel   # Constraint- only intel cpu
```

```
#SBATCH -p main    # Partition
#SBATCH --qos main  # Quality of service
#SBATCH -o lammps_sim_out-%J.txt  # STDOUT Out file
#SBATCH -e lammps_sim_out-%J.txt  # Error file file
#SBATCH -t 5                      # time in minutes

cd ~/lammpstest                   # Moving to the test diectory

mpirun lammps -in in.flow.pois    # Run the lammps command
```

Now, you can schedule the job with sbatch command.

The output file will be a txt file will processed information.

Where to find help?

If you are stuck on some part or need help at any point, please submit a help request through the HPC portal.

https://ua-app01.ua.edu/researchComputingPortal/public/oitHelp

Resources:

https://oit.ua.edu/services/research/research-computing-support/mpi-on-hpc/