

# Protocol run LAMMPS in hipatia cluster

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## 1 Introduction

1. Open the terminal and go to the folder of simulations. eg. `cd Downloads`
2. write: `ssh username@hpc.bcamath.org -p6556`
3. Insert password

### 1.1 Interactive mode:

Write in the terminal

1. `salloc -n 8 -time=1:00:00 -p medium` (8 nodes in 60 minutes) (User changes from `username_@xcat` to the name of the node `username_@n001`)
2. `squeue -u username` (to check the running processes)
3. check if the folder and files are in the cluster.
4. `cd FolderName` (folder)
5. `ml LAMMPS/29Oct20-foss-2019b-Python-3.7.4-kokkos-sdpd-dynamicD` (open the library of LAMMPS \*\*)
6. `mpirun -n 8 lmp - mpi<in.mobility` (To run the simulation)
7. `exit (username_@xcat)`
8. `exit` (for the cluster)
9. copy the results in your computer.

To copy the folder from your computer to the cluster you need to exit your login in the cluster, go to the path of your folder and write in the terminal:

1. `rsync -arv -e "ssh -p 6556" FolderName username@hpc.bcamath.org:/home/username/`

On the other hand, if you want to copy the results of the simulation on your computer you need to write the next instruction in the terminal:

1. `sync -arv -e "ssh -p 6556" username@hpc.bcamath.org:/home/username/FolderName/*`  
./ (copy the results to your computer)

Do not forget be located in the path of the folder where you want to copy or synchronize the files.

## 1.2 Batch mode:

Write in the terminal

1. Go to the folder where are the files you will run
2. `sbatch script.hipa` (To run the simulation if you have a script file with all the information about the simulation)
3. `squeue -u username` (to check the running processes)
4. `exit` (for the cluster)
5. `rsync -arv -e "ssh -p 6556" username@hpc.bcamath.org:/home/username/FolderName/*`  
./ (copy the results to your computer )

\* change username for your actual user name

\*\* make sure that the library that you use is installed in the cluster. Go to <https://docs.google.com/document/d/1EsA2H5KZh6AbmcG5ZNmdbipaa76lj1YDaBuW0bcgeck/edit>. for more information or write in the terminal: `module spider name of the library`