

- Once you have installed OpenMM and copied the data, you can simply run the python script on the login terminal
- However, this is not the way that you're supposed to do things
- If you try to run a big calculation on the login terminal the system administrators will get mad at you!

```
(openmm) br006:[~]: python -m simtk.testInstallation

OpenMM Version: 7.4.1
Git Revision: 068f120206160d5151c9af0baf810384bba8d052

There are 2 Platforms available:

1 Reference - Successfully computed forces
2 CPU - Successfully computed forces

Median difference in forces between platforms:

Reference vs. CPU: 6.30481e-06

All differences are within tolerance.
(openmm) br006:[~]: ls
scripts  software  ubq-md
(openmm) br006:[~]: cd ubq-md/
(openmm) br006:[~/ubq-md]: ls
1ubq.pdb  MD_ubq.py
(openmm) br006:[~/ubq-md]: python MD_ubq.py
Minimizing...
Running Production...
#"Progress (%)" "Step" "Potential Energy (kJ/mole)" "Temperature (K)"
"Speed (ns/day)" "Time Remaining"
10.0% 100 -12937.54104464231 178.8691182900329 0 --
20.0% 200 -12786.424474924024 206.88709731573758 21.9 0:06
30.0% 300 -12425.520220420438 214.78270910359848 21.8 0:05
40.0% 400 -12333.981042607265 242.67256593500656 21.8 0:04
50.0% 500 -12170.023875048062 252.83736423813997 21.8 0:03
60.0% 600 -12043.26256936375 262.77890676191413 21.7 0:03
70.0% 700 -12022.84441006196 274.6817644781113 21.8 0:02
80.0% 800 -11904.676295196514 279.1694256963495 21.8 0:01
90.0% 900 -11873.317454425185 274.09491413581435 21.7 0:00
100.0% 1000 -11727.128648981274 275.21880048454915 21.7 0:00
Done!
```

# Submitting jobs to Bridges

- As described in the Bridges user guide under “Running Jobs”, you can submit a job to the cluster using a batch script
- Bridges uses the SLURM (Simple Linux Utility for Resource Management) scheduler
- A batch job consists of
  - a line that describes the shell, e.g. `#!/bin/bash`
  - SLURM directives that describe job properties, starting with `#SBATCH`
    - many directives can be command-line arguments, but it is generally better to save job properties into the job script
    - other schedulers will have different directives
  - executable commands, details of which will depend on the shell
  - optionally, comments after `#`