- 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 `#’