- 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%
                -12786.424474924024
                                                                        0:06
        200
                                        206.88709731573758
                                                                21.9
30.0%
                                        214.78270910359848
        300
                -12425.520220420438
                                                                21.8
                                                                        0:05
40.0%
                                                                        0:04
        400
                -12333.981042607265
                                        242.67256593500656
                                                                21.8
50.0%
        500
                                                                        0:03
                -12170.023875048062
                                        252.83736423813997
                                                                21.8
60.0%
                                                                21.7
       600
                -12043.26256936375
                                        262.77890676191413
                                                                        0:03
                                                                        0:02
70.0%
                -12022.84441006196
                                        274.6817644781113
                                                                21.8
80.0%
        800
                -11904.676295196514
                                        279.1694256963495
                                                                        0:01
                                                                21.8
90.0%
                                        274.09491413581435
        900
                -11873.317454425185
                                                                        0:00
                                                                21.7
                                        275.21880048454915
100.0%
       1000
                -11727.128648981274
                                                                21.7
                                                                        0:00
Done!
```

Submitting jobs to Bridges

- As described in the <u>Bridges user guide</u> 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 `#'