

- To actually run OpenMM, you need to invoke a Python script.
- To invoke the script, enter the following commands
 - ``cd ~/Desktop/OpenMM'`, which changes your current directory to the directory where the files are
 - `'ls'` lists the contents of the current directory. It isn't 100% necessary but useful to check.
 - ``python MD_ubq.py'` actually runs the script

```
(openmm) Minh-IIT-MBP2018: [~]: cd ~/Desktop/OpenMM
(openmm) Minh-IIT-MBP2018: [~/Desktop/OpenMM]: ls
1ubq.pdb    MD_ubq.py
(openmm) Minh-IIT-MBP2018: [~/Desktop/OpenMM]: python MD_ubq.py
```

Input files can also be downloaded from github:

https://github.com/daveminh/Chem456/tree/master/static_files/tutorials/ubq-md

- When you run the script, you will see some output to the console. This is mostly from the StateData reporter
 - Notice that the potential energy goes slightly up. This is because we started with a minimized structure.
- If you type `ls` again, you will see that the simulation created two files
 - ubq_mod.pdb - the model that includes hydrogen but not water
 - trajectory.dcd - the actual simulation data

```
(openmm) Minh-IIT-MBP2018:[~/Desktop/OpenMM]: python MD_ubq.py
Minimizing...
Running Production...
#"Progress (%)" "Step" "Time (ps)" "Potential Energy (kJ/mole)" "Temperature (K)" "Speed (ns/day)"
Time Remaining"
10.0% 100 0.200000000000000015 -12936.42476230517 183.51751922475094 0 --
20.0% 200 0.40000000000000003 -12646.180945641867 208.17988992042834 66.3 0:02
30.0% 300 0.60000000000000004 -12391.382319417527 222.92731255729387 63.9 0:01
40.0% 400 0.80000000000000006 -12397.931712869551 252.91336736415292 63.2 0:01
50.0% 500 1.00000000000000007 -12164.42101471391 261.4505010540196 63.7 0:01
60.0% 600 1.20000000000000008 -11959.584803213324 267.99278996281504 63.9 0:01
70.0% 700 1.4000000000000001 -11810.354813818332 278.89717139432463 64.1 0:00
80.0% 800 1.60000000000000012 -11819.44354535209 280.87644275577924 64.5 0:00
90.0% 900 1.80000000000000014 -11761.649241585736 281.12817290253514 64.6 0:00
100.0% 1000 2.00000000000000013 -11685.676062540104 281.4727076092732 64.9 0:00
Done!
(openmm) Minh-IIT-MBP2018:[~/Desktop/OpenMM]: ls
1ubq.pdb MD_ubq.py trajectory.dcd ubq_mod.pdb
(openmm) Minh-IIT-MBP2018:[~/Desktop/OpenMM]:
```