

Running OpenMM

- 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