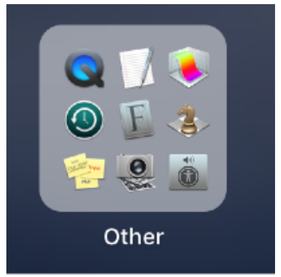
2/18/2020 Week 6 Module 1
Running molecular dynamics on a remote computer

- Useful molecular dynamics simulations and other scientific calculations often require too much computer power to run on a local laptop or desktop
- In this module, you will learn how to
  - log into a remote computer
  - install OpenMM on the remote computer
  - transfer data to and from a remote computer
  - submit a calculation to a queue on a computing cluster
- We will use remote computers belonging to XSEDE, the “Extreme Science and Engineering Discovery Environment”, an organization that manages computing resources for open science throughout the United States

Review: The UNIX Terminal

- Predecessor and very similar to the terminal used in
  - LINUX - many scientific computing clusters
  - Mac OS X - this lab and many of your own laptops/computers
- Useful for
  - accessing programs that run with a command line interface (CLI)
  - automation

- To start the terminal on a Mac:



- I actually usually use another program: