Installing MD analysis packages w/ conda

- conda create --name mdanalysis
- conda activate mdanalysis
- conda config --add channels conda-forge
- conda install jupyter pandas mdanalysis pymbar
  - juypter - for interactive coding notebooks
  - pandas - for data analysis
  - mdanalysis - for loading and analyzing MD trajectories
  - pymbar - for calculating free energies. also contains equilibration detection.

What is equilibration?

- The early part of a simulation is biased by the initial configuration
  - macromolecule structures start in a local minimum
  - water and ions are placed somewhat arbitrarily
  - box size is probably too large
- Equilibration is the time a system takes to reach a representative configuration
- Generally, simulation results from the equilibration period are ignored
- The samples actually used to calculate averages are known as the production

- See Equilibration.ipynb, which illustrates these points for a simulation of ubiquitin.