3/5/2020 Week 8 Module 2
Analysis of molecular dynamics simulations 2

- This module will consist of
  - an explanation of dimensionality reduction, conformational clustering, and Markov State Models in the analysis of biological MD
  - a tour of an analysis of a ubiquitin simulation
    - based on the python package MDAnalysis
    - that you can follow for your own system
- At the end of this module, you should be able to answer the following questions:
  - What is dimensionality reduction? What is one way to do it?
  - What is clustering and why is it useful? What is one way to do it?
  - What are Markov State Models and why are they useful?
- Hopefully you can modify the scripts that I used to analyze your own systems.
- Let me know if you feel that the class is going too quickly

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.

- If you want to try Markov State Models, you may need to downgrade python first
  - conda install python=3.7
  - conda install pyemma
    - pyemma - for Markov state models