3/3/2020 Week 8 Module 1
Analysis of molecular dynamics simulations 1

- This module will consist of
  - an explanation of key principles in the analysis of biological MD simulations
  - 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 MD used to calculate?
  - What is equilibration? How is the equilibration time determined?
  - Why is structural alignment helpful? How is it done?
  - What is principal components analysis? What is one way to do it?
  - What is clustering and why is it useful? What is one way to do it?
- You should also be able to visualize a MD trajectory in VMD. Hopefully you can modify the scripts that I used to analyze your own systems.

What is MD used to calculate?

- MD simulations may be used to
  - predict events or sequence of events that are physically possible
  - estimate statistical averages of
    - configurational properties, e.g.
      - average distance between two residues
      - histogram of an angle between three domains
      - populations of certain conformations
    - rates
- Statistical estimation is based on the assumption of ergodicity - that the time average is equal to the ensemble average