How is equilibration time determined?

- Arbitrarily
- Once a key property is stabilized
- By maximizing the effective sample size [Chodera, 2016]
  - A short equilibration leads to a long estimate of the time for the sample to be independent
  - A long equilibration reduces the number of samples
- Equilibration time
  - may look different for different properties
  - if properties are independent, slow equilibration of one may not affect estimation of another

Structural alignment

- Other than identifying equilibration time, structural alignment is usually one of the first tasks of MD analysis
- Why?
  - In most MD simulations, molecules freely diffuse around the box
  - We are usually
    - uninterested in the overall translation and rotation,
    - interested in fluctuations relative to the macromolecule
- Alignment is often based on a rigid-body translation and rotation to minimize the root mean square deviation (RMSD)

- See Alignment.py, which performs a structural alignment for a series of simulations of ubiquitin and outputs a trajectory of the protein by itself.