

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.

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