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

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.