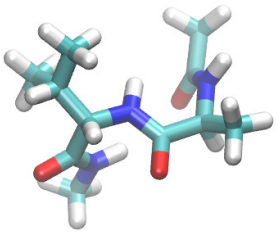

Project: MSM comparison of Ac-AP-NHMe and Ac-AA-NHMe dimer

B. Trendelkamp-Schroer, M. Scherer, F. Paul, and F. Noe

February 24, 2015

The relevant coordinates for the two dimers are given in terms of the Alanine dihedral angles, (ϕ_A, ψ_A) and the Proline dihedral angles (ϕ_P, ψ_P). We want to build MSMs to compare the dynamics of the two dimer-molecules.

For the Ac-AP-NHMe molecule

- Use the provided file `dihedral_AP.npy` containing the dihedral angle trajectory $(\phi_A, \psi_A, \phi_P, \psi_P)$ with a time-step of $1ps$.
- Plot (ϕ_A, ψ_A) and (ϕ_P, ψ_P) trajectories seperately and compare your plots to the stationary distribution for Alanine-Dipeptide from the tutorial. What do you observe?
- Define a coarse discretization for the system. It might be helpful to first obtain a discretized trajectory for each monomer and to combine them in a second step.
- Build a reversible MSM and compute time-scales.

Repeat the above for the Ac-AA-NHMe molecule using the dihedral angles in `dihedral_AA.npy`. Compare the computed time-scales for both dimers. What do you find? Visualize the dominant right eigenvectors. What can you say about the slowest processes in the system?