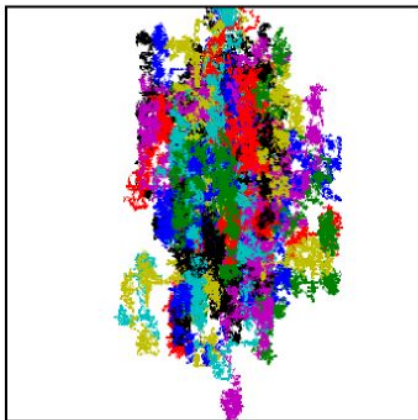
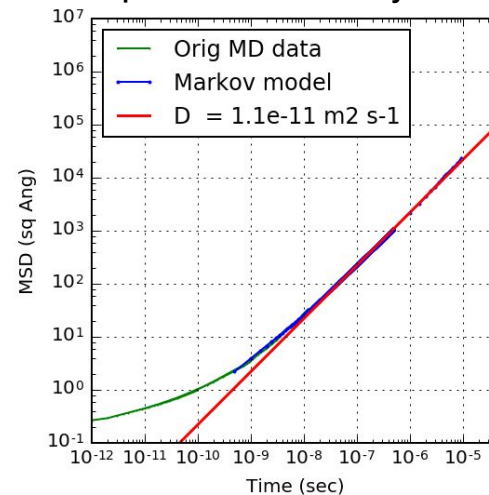


Molecular dynamics simulation trajectories

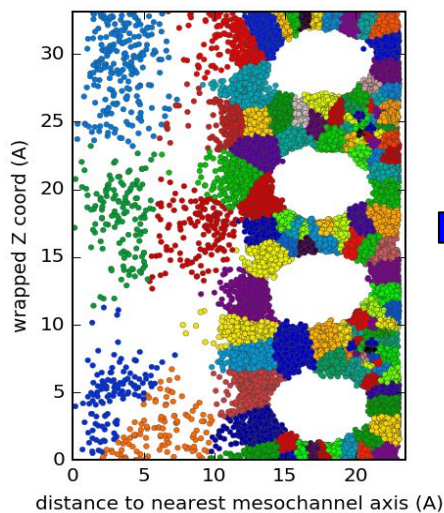


Data is insufficient

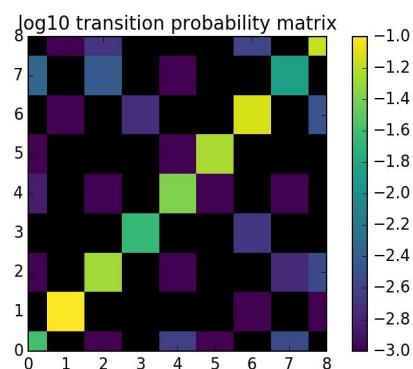
Diffusion estimate from mean squared displacement of trajectories



Discretization of data in a relevant coordinate system



Markov state model



MCMC extended trajectories

