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Non-Markovian Dynamic Models for Studying Protein Conformational Changes

Protein's dynamic transitions between metastable conformational states play an important role in numerous biological processes. Markov State Model (MSM) built from molecular dynamics (MD) simulations provides a useful approach to study these complex dynamic transitions, but it is challenging to build truly Markovian models due to the limited length of lag time (bound by the length of relatively short MD simulations). In this talk, I will introduce our recent work on developing non-Markovian dynamic models based on the Generalized Master Equation (GME) theory that encodes the dynamics in a generally time-dependent memory kernel, whose characteristic decay time scale corresponds to the kernel lifetime. We show that GME methods can greatly improves upon Markovian models by accurately predicting long timescale dynamics using much shorter MD trajectories on complex conformational changes.