Investigation Conformational Changes of Biological Macromolecules Using Kinetic Network Models

Xuhui Huang
The Hong Kong University of Science and Technology

Simulating biologically relevant timescales at atomic resolution is a challenging task since typical atomistic simulations are at least two orders of magnitude shorter. Markov State Models (MSMs), a kinetic network model, built from molecular dynamics (MD) simulations provide one means of overcoming this gap without sacrificing atomic resolution by extracting long time dynamics from short MD simulations through the coarse graining on the phase space and time. In this talk, I will demonstrate the power of kinetic network models by applying it to simulate the complex conformational changes, that occurs at tens of microsecond timescales for a large RNA transcription complex (close to half million atoms). In the second part of my talk, I will introduce a new efficient dynamic clustering algorithm for the automatic construction of MSMs for multi-body systems. We have successfully applied this new algorithm to model the protein-ligand recognition and hydrophobic collapse processes that occur at a mixture of different timescales.