Efficiently extracting thermodynamics and kinetics from molecular simulation data at multiple thermodynamic states

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I will present novel methods based on Markov modeling for extracting statistical information (thermodynamics and kinetics) from molecular simulation data that has been generated at multiple thermodynamic states. Such data may be obtained from enhanced sampling protocols, such as umbrella sampling or replica-exchange dynamics, and by mixing one of these protocols with direct molecular dynamics data. Here I will propose ways to optimally extract information from such data, including the reconstruction of the kinetics of rare events that are not directly sampled in the data. An application of our approach is the estimation of rare unbinding kinetics of protein-ligand complexes when only the more frequent binding process can be sampled in direct MD simulations.