Optimal control of molecular dynamics using Markov state models

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The effective dynamics of molecular system can be characterized by the switching behavior between several metastable states, the so-called conformations of the system that determine its functionality. Steering a molecular system from one conformation into another one on the one hand is a means to controlling its functionality while on the other hand it can be used to gather information about transition trajectories.
This talk considers optimal control problems that appear relevant in steered molecular dynamics (MD). It will be demonstrated how the associated Hamilton-Jacobi-Bellman (HJB) equation can be solved. The main idea is to first approximate the dominant modes of the MD transfer operator by a low-dimensional Markov state model (MSM), and then solve the HJB for the MSM rather than the full MD. We then will discuss whether the resulting optimal control process may help to characterize the ensemble of transition trajectories.
The resulting method will be illustrated in application to the maximization of the population of alpha-helices in an ensemble of peptides.