Simple models for molecular dynamics:

Markov state models and beyond

Jan-Hendrik Prinz

Computational Molecular Biology Group, Freie Universität Berlin, Arnimallee 6, 14195 Berlin

In recent years Markov State Models (MSMs) have gained much popularity as a simple way to describe the dynamics of large biomolecules, especially proteins. Once a model has been parametrized from simulated or experimental data it allows for a fast and efficient computation of various key properties of interest like relaxation timescales, metastable subsets, reaction pathways and other observables that can be compared to experimental results. One mayor problem for the MSM approach is the necessity of a good discretization of state space, where *good* refers to the ability of the discretization to capture the metastable structure. Especially for experimental data this requirement can often *not* be fulfilled and MSMs fail to describe the observed dynamics accurately. This leads to new concepts like Projected Markov Models (PMMs) and Observable Operator Models (OOMs) that try to keep the simplicity of the MSM approach while not being affect by poor discretizations or uncorrelated noise.

The talk will give an introduction into MSMs and how they can be used to describe the dominant / long-term dynamics of biomolecules. The possibilities and problems of this approach are outlined and potential solutions using PMMs and OOMs are shown.

Thursday, October 31st, 2013
16:00 s. t.
ICP building, Allmandring 3, Seminar room 1.079