Recent progress in multiscale molecular dynamics simulation

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Multiscale modeling techniques allow to simulate larger systems and longer time scales by reducing the level of detail in the model where and when possible. In this talk I will present two multiscale methods that we have recently developed.

The first method is path-metadynamics, which allows us to sample activated processes, such as chemical reactions, that take place on a time scale that is much longer than the accessible time of a straightforward molecular dynamics simulation. Path-metadynamics determines the most-likely reaction path as a function of (many) selected coordinates and obtains the free energy profile along this reaction path. As an example, I will show its application to unravel the light-activated conformational transition in photoactive yellow protein.

The second method is adaptive multiscale molecular dynamics, which we developed to study the interesting parts of a molecular system in atomistic detail, while including the environment with a reduced, coarse-grain, model. The boundaries of the atomistic/coarsegrain regions are open and the molecules that diffuse over adapt their resolution on the fly. I will briefly discuss the statistical mechanical consequences of such hybrid multiscale modeling and show its application to model the swelling of a polymer.

Thursday, January 24th, 2013
16:00 s. t.
ICP building, Allmandring 3, Seminar room 1.079