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# Efficient Simulation in Protein Modelling and Non-equilibrium Processes

The behavior of a molecule is described by the Boltzmann distribution in conformation space. In classical molecular dynamics a trajectory describes the time dependent dynamics of a protein. Thereby the time step is confined to the fastest oscillation of the covalent bonds and thus shortens the absolute simulation time. Contrary, events which are relevant for protein design, such as protein folding occur only after comparably long time. Thus we have a time gap, between the fastest simulation which determine the maximum possible simulation time and the rare events which have a great impact on the configuration of the protein. Additionally with increasing size of the molecule the dimension of the corresponding conformation space and thus the computational complexity growths.
Consequently one seeks for methods which extract the relevant information out of the simulation data with less computational complexity. This is the basic concept of the coarse graining techniques. These methods take advantage of the fact, that the rare events can be "detected" by mathematical methods. In the last few decades various coarse graining techniques have been developed in order to bridge this time gap in biological processes. Here, we focus on conformation dynamics, where in contrast to classical MD one is interested in the identification of metastable states and transition probabilities. Moreover meshfree methods are introduced for a suitable discretization of the conformation space in high dimensions.
On this basis, we focus on the force simulation of non equilibrium processes which play an important role in protein miss folding diseases such as Alzheimer's disease. Furthermore, we motivate how results from computer simulation and experimental data from laboratory can be combined in a meaningful way.