Iris Antes
Technical University of Munich
e-mail: antes@wzw.tum.de

Hierarchical approaches for the investigation of biomolecular recognition

One of the major bottlenecks for the computational description of biological processes on the molecular and atomistic level is the limitation in the time scale and system size which can be treated by the existing theoretical methods. Much research has been devoted to this problem and many advanced biophysical methods have been developed for this task. Most of them are, however, very time consuming and not applicable to applications for which very complex systems must be investigated and if many different situations must be investigated simultaneously, like in computational drug or protein design. To be able to deal with such applications, we develop hierarchical models, which combine very efficient, discrete methods from computational biology with more demanding continuous biophysical approaches. In the presentation an overview over the methodology will be presented together with examples for their practical applications.