Abstract:

The macroscopic dynamics of DNA molecule is mainly characterized by the existence of biomolecular conformations which can be understood as metastable large scale structures, i.e. geometries which are persistent for long periods of time. The mathematical models of DNA dynamics should be able to represent the heterogeneity of the underlying physicall processes and be consistent w.r.t the description of conformational changes. A novel method for the identification of the most important conformations from molecular dynamics time series by means of Hidden Markov Models (HMMs) with output behavior given by stochastic differential equations (SDEs) will be presented. The application of the HMM-SDE model for the construction of the coarse--grained models and identification of sequence-dependant elasticities will be demonstrated . The combination of TRAIL (Trapezoidal Rule for Adaptive Integration of Liouville dynamics) method with HMM-SDE approach can be used for the propagation of derived coarse models. This will be exemplified with application to a well-known Micheilis--Menten kinetics.