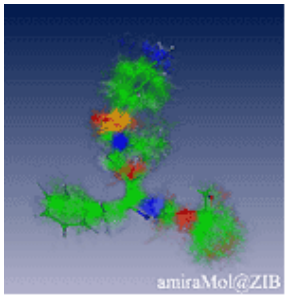
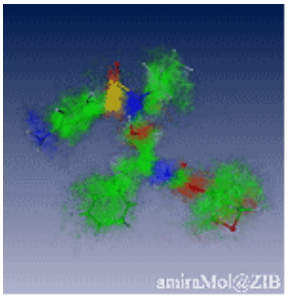
Markovian Systems

Markovian Systems / Metastability & Model Reduction

There are many problems in physics, biology, medicine, where the length and time scales of interest remain entirely beyond the computational capacity currently available, and will remain out of reach in the foreseeable future. As a consequence, there is an increasing need for simplified, reduced descriptions.
Reduced -order models may provide insight and numerical simulations for larger length scales and longer time scales, but of course at the cost of discarding some level of detail. Instead of simply neglecting some degrees of freedom, one is rather interested in reduced models that incorporate into their dynamical behaviour the effective influence of the neglected coordinates.
The aim of the project is to develop mathematical tools and numerical algorithms for the identification and efficient simulation of reduced model systems.





In cooperation with the Bio Computing Group (http://biocomputing.mi.fu-berlin.de) (FU Berlin) and the Molecular Dynamics Group (http://www.zib.de/Numerik/DrugDesign/index.en.html) (ZIB) we develop novel mathematical methods for the identification of metastable behaviour in Markovian systems, in particular in application to the conformation dynamics of drug-like molecules. Furthermore, we cooperate with A. Stuart (Warwick) and S. Meyn (Urbana/ Champaign) on the derivation and theoretical justification of reduced models.

 http://compphysiol.math.uni-potsdam.de/