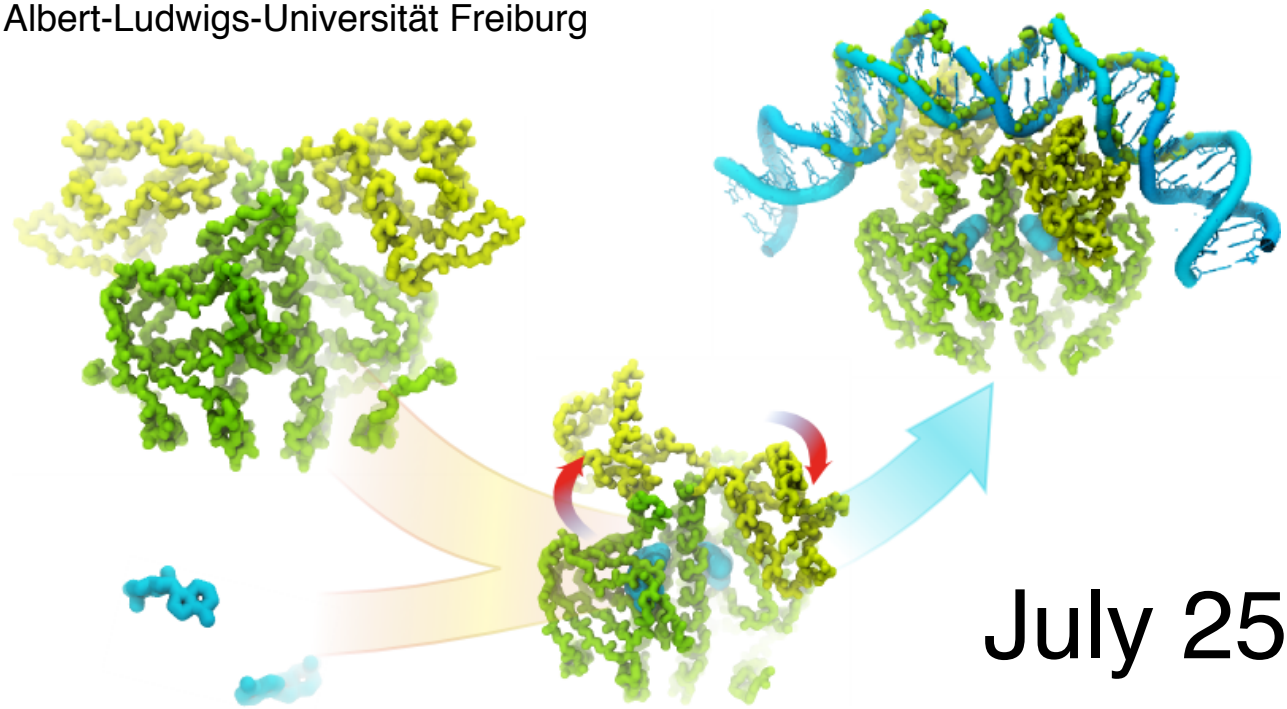
Physikalisches Institut

Albert-Ludwigs-Universität Freiburg



July 25

Markov models of molecular conformation dynamics

Frank Noé

FU, Berlin

Biomolecular molecular kinetics deals with finding the number and structural definition of metastable states, the relaxation timescales arising from the transitions between them, and the assignment of structural rearrangements to these timescales. It is challenging to extract such kinetic information from either simulations or experiments, due to such problems like the sampling problem, the problem of analyzing huge data sets, limited observability of coordinates, etc. I will talk about some recent ideas and trends in the model of essential molecular kinetics with Markov models, including the following topics: 1) How can we efficiently explore state space in molecular simulations, in order to initialize Markov modeling? 2) What is required for a "good" Markov model of the data, and why? Comparison of several approaches (many states, few metastable states, core approach) 3) How can we extract Markov models from single-molecule experimental trajectories where observables may overlap? 4) Some remarks on analysis (Transition path theory etc).

Molecular Dynamics Seminars 2012

Seminar Room of Gustav Mie Haus, Ground Floor, 16:15

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SCHOOL OF SOFT MATTER RESEARCH

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