Freitag, 25. November 2016, 16.00 Uhr
Ort: Raum 108, Arnimallee 6, 14195 Berlin
Disputation über die Doktorarbeit von
Herrn Benjamin Damian Trendelkamp-Schroer

Thema der Dissertation:
Reversible Markov State Models

Thema der Disputation:
Statistical reweighting

Die Arbeit wurde unter der Betreuung von Prof. Dr. F. Noé durchgeführt.

Abstract: The rare occurrence of conformational changes on timescales accessible by molecular dynamics simulations results in a sampling problem. Equilibrium expectation values cannot be accurately estimated by simulations, so that interesting thermodynamic properties of the molecular system remain inaccessible. To overcome the sampling problem statistical reweighting methods can be used to efficiently estimate the desired expectation values from simulations that sample a set of artificial ensembles.

The talk will focus on two reweighting methods: The weighted histogram analysis method (WHAM) [1] and the transition based reweighting analysis method (TRAM) [2,3]. While WHAM is a well established method, TRAM has been recently developed to overcome limitations, that make WHAM unsuited for the study of molecular systems. TRAM leads to a nonlinear constrained optimization problem that is difficult to solve and exhibits a problematic scaling behavior. A dual problem with better analytic properties and dramatically improved scaling can be derived. But, the fixed-point iteration employed for the solution of the dual problem can take a long time to converge. It will be shown that a Newton type method can be used to significantly improve the time required for a solution of the TRAM problem.


Die Disputation besteht aus dem o. g. Vortrag, danach der Vorstellung der Dissertation einschließlich jeweils anschließenden Aussprachen.

Interessierte werden hiermit herzlich eingeladen
Der Vorsitzende der Promotionskommission
Prof. Dr. F. Noé