

FREIE UNIVERSITÄT BERLIN Fachbereich Mathematik und Informatik

Promotionsbüro, Arnimallee 14, 14195 Berlin

DISPUTATION

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.

[1] A. M. Ferrenberg and R. H. Swendsen. Optimized Monte Carlo data analysis. Phys. Rev. Lett. 63, 1195 (1989).

[2] H. Wu, A. Mey, E. Rosta, and F. Noe. Statistically optimal analysis of state-discretized trajectory data from multiple thermodynamic states. J. Chem. Phys. 141, 214106 (2014).

[3] H. Wu, F. Paul, C. Wehmeyer, and F. Noe. Multiensemble Markov models of molecular thermodynamics and kinetics. Proc. Natl. Acad. Sci. USA 113(23), 3221-3230 (2016).

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