A U S H A N G

FREIE UNIVERSITÄT BERLIN

Fachbereich Mathematik und Informatik

Promotionsbüro, Arnimallee 14, 14195 Berlin

D I S P U T A T I O N

Freitag, 28.04.2023, 15:00

Ort: Hörsaal B (0.1.01)

(FB Physik, Arnimallee 14, 14195 Berlin)

Disputation über die Doktorarbeit von

Herrn Andreas Mardt

Thema der Dissertation:

Deep learning of the dynamics of complex systems with its applications to biochemical molecules

Thema der Disputation:

From Complexity to Clarity: Understanding Protein Dynamics with Markov State Models

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

Abstract: Markov State Models (MSMs) are a popular method for analyzing complex molecular dynamics simulations and capturing long-timescale kinetics. In MSMs, the dynamics of a system are discretized into a set of states, and the transitions between these states are modeled as a Markov process. In my first talk, I will highlight keystone developments to their application to modelling protein-protein or protein-ligand interaction. The main emphasis will be on the variational approach to conformational dynamics (VAC), which has enabled the MSM building process to become more structured and unbiased, shifting away from being dependent on expertise. In my second talk I will explore how a generalization of this approach can further facilitate the building of such models with the assistance of neural networks.

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