

A U S H A N G

FREIE UNIVERSITÄT BERLIN

Fachbereich Mathematik und Informatik

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DISPUTATION

Donnerstag, 30. Juni 2022, 10:15 Uhr

[WebEx](#)

Disputation über die Doktorarbeit von

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Thema der Dissertation:

Modelling Observations of Dynamical Systems with Memory

Thema der Disputation:

Robust numerical schemes for the approximation of the memory kernel in the Generalized Langevin Equation

Die Arbeit wurde unter der Betreuung von **Prof. Dr. C. Schütte** durchgeführt.

Abstract: Modelling the time-evolution of physical systems with many degrees of freedom can quickly become both analytically and numerically infeasible. Therefore, it is often advised to model the quantities of the system that are relevant to the modeller directly. It is well-known that projecting a dynamical system onto such observed variables introduces memory effects in the observed dynamics unless certain special conditions are met. The Mori-Zwanzig formalism allows the construction of an equation for the observed dynamics consisting of a Markovian term denoting the best memoryless prediction for the time-derivative of the observed variables, an inaccessible noise term and a memory term given by the integral over a typically complex function. Together, for time-continuous systems, these terms compose the so-called Generalized Langevin Equation (GLE). While in some cases the Markovian term can straightforwardly be modelled using statistical assumptions on the non-observed variables of the dynamics, the handling of the memory term requires certain approximation steps for which several numerical approaches exist. In this talk, a specific class of these approaches, defined predominantly by the Netz-group from FU Berlin, will be presented. It extracts the memory term from data and approximates it by a parametric function. This is done in a way that admits both a ready numerical simulation of the ensuing approximated GLE and an interpretation in regard to time scales of the observed dynamics. The method shows especially promising results in physical systems in which the observed dynamics show metastable behaviour.

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. C. Schütte