Seminar:
Stochastic processes and Reaction Rate Theory

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Modeling and Simulation of Complex Processes
Computational Molecular Design

18 April 2024

Important information

- Date: Thursday
- Time: 10:15 am - 11:45 am
- Location: Arnimallee 6, SR 025/026

Structure of the seminar

- 5 weeks (18., 25. April; 2., 16. 23. May): Lectures
- 3 weeks (30. May; 6., 13. June): Projects (working alone)
- 3 weeks (20., 27. June; 4. July): Projects (working in class with the lecturer)
- 2 weeks (11., 18. July): Presentation of results

- Introduction to reaction rate theory - Kramers theory
- Transfer operator approach
- SqRA of the infinitesimal generator
- Robust Perron Cluster Cluster Analysis (PCCA+)
- Invariant subspaces of Koopman operators learned by a neural network (ISOKANN)

Projects

- Kramers theory: Study the Langevin dynamics of a one-dimensional problem, calculate the rates applying the Kramers theory, verify under which conditions the Kramers theory holds.
- SqRA: Study the overdamped Langevin dynamics of an N-dimensional problem with SqRA and Langer theory.
- PCCA+: Provided a rate matrix, implement PCCA+ to study the metastable states of the system.
- ISOKANN: Implement ISOKANN to study metastable states and estimate the transition rates of a molecular system.

Literature

- Lecture notes.
- Articles provided by the lecturer.
- Chapters from *Baron Peters, Reaction Rate Theory and Rare Events Simulations* provided by the lecturer.