Universität Stuttgart
Cluster of Excellence EXC 2075 „Data-Integrated Simulation Science“

"Calculating Free Energy Differences from Molecular Simulation: Theory and Practical Applications“

Graduate Academy SimTech

GS Seminar by
Prof. Niels Hansen

Description: The free energy difference between two states of a (bio)molecular system is one of the central quantities of interest in (bio)molecular simulation. A maze of computational techniques to calculate free energies is nowadays available that differ in efficiency and accuracy.

However, most of them are rooted in a few basic ideas. In this lecture state of the art methods to calculate free energy differences in the context of classical molecular dynamics simulations will be discussed in light of these basic ideas. Emphasis is given to both a theoretical analysis as well as issues of practical implementation.

The two main types of free energy calculations, changes in the Hamiltonian (so-called alchemical perturbations) and changes in the configuration will be covered. Finally, the participants will present and discuss their own free-energy related research questions.

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Language: English

Date: To be discussed with the participants

Time: To be discussed with the participants

SWS: 2

ECTS: 3

Proof of attendance: Regular presence and active participation in exercises and presentations

Please register via email.

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