Diszipline Forum
of the post graduate program
in the SFB 765

Molecular Dynamics Simulation

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Location: Seminar Room 26.07, Arnimallee 22

Abstract:
The method of Molecular Dynamics (MD) is one of the principal tools in the theoretical study of biological molecules. Using classical Newton equations of motion, this computational method calculates the time dependent behavior of a molecular system using empirical and/or quantum mechanical forcefield parameters. It now is routinely used to investigate the structure, dynamics and thermodynamics of biological molecules and their complexes, but also helps in the determination of structures from x-ray crystallography and from NMR experiments.
However, limited computation power and the fact that the relevant states only cover small parts of the phase space require efficient algorithms and well posed questions before starting the simulation process, as well as methods of evaluating the obtained data.
In this seminar, we will give a brief overview of the MD method and present some examples from the membrane transport, protein folding and ligand binding. We also introduce our concept of how to apply MD simulations to interactions between biological membranes at the nanoscale where the correct chemical potential of the solvent becomes a challenging task.