GSS Summer School 2017

Molecular Dynamics - Structure and Dynamics of Water

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In this exercise you will perform classical molecular dynamics (MD) simulations, *i.e.* the Newtonian equations of motion will be solved iteratively for a many-particle system. In classical MD, the interactions between particles are described using molecular mechanics force fields. This is an approximation, because the interactions between particles can be fully described only by solving the (time-independet) Schrödinger equation (referred to as *ab initio* MD). However, a force field has advantages over quantum mechanical methods: (1) it is very time-efficient and allows the simulation of systems up to the order of 10^6 in reasonable time, (2) for systems such as solvated proteins, membranes or DNA usually a classical description is sufficient to analyze mechanistic insights as well as structure and dynamics of molecules.

You will learn how to generate a topolgy for a water box and to prepare it for the final production simulation. From the production simulation you will obtain information on the structure and dynamics of the system. The MD program package `GROMACS` will be the tool to perform all steps of this course.