FSI3450 Advanced Molecular Dynamics 7.5 credits

Avancerad molekyldynamik

This is a translation of the Swedish, legally binding, course syllabus.

Establishment

Course syllabus for FSI3450 valid from Autumn 2011

Grading scale

G

Education cycle

Third cycle

Specific prerequisites

• Basic knowledge of statistical mechanics / thermodynamics

(the course includes a brief introduction to Molecular Dynamics and force fields)

Language of instruction

The language of instruction is specified in the course offering information in the course catalogue.

Intended learning outcomes

After completion of the course, the student should be able to:

- set up simulations of liquids, polymers and proteins
- analyze structural and dynamic properties
- assess the quality of sampling and be aware of methods to improve sampling
- set up free energy calculations
- apply systematic coarse-graining

Course contents

This course treats advanced molecular dynamics (MD) methodology for classical simulations of liquids, polymers and proteins. MD simulations provide atomistically detailed information on structural and dynamic quantities, but often at a high computational cost. As vibrations of atoms need to be captured, time steps are in the order of femtoseconds, whereas the time scales of interest are often in the microsecond to second range. This has three main implications. Efficient software and hardware is required, using for instance stream computing (on e.g. GPUs). You always need to carefully check the convergence of properties of interest. And if convergence can not be reached, you might need to use methods to improve sampling, such as free energy calculations and coarse-graining. These topic will be covered in lectures, reading of literature and computer labs.

Course literature

- D. Frenkel & B. Smit, Understanding Molecular Simulation
- H.J.C. Berendsen, Simulating the Physical World
- Selected articles

Examination

Based on recommendation from KTH's coordinator for disabilities, the examiner will decide how to adapt an examination for students with documented disability.

The examiner may apply another examination format when re-examining individual students.

If the course is discontinued, students may request to be examined during the following two academic years.

Other requirements for final grade

- Computer Labs using the Gromacs simulation package
- Presentation of projects which can be adapted to the particular interests of students

Ethical approach

- All members of a group are responsible for the group's work.

- In any assessment, every student shall honestly disclose any help received and sources used.

- In an oral assessment, every student shall be able to present and answer questions about the entire assignment and solution.