

Syllabus for the course Monte Carlo and Molecular Dynamics Tools, NTF008F

Swedish title: Monte Carlo- och molekylodynamikverktyg

The course syllabus was confirmed by the Faculty board for graduate studies 4 June 2019. The course is in the third cycle and amounts to 7.5 credits.

The course syllabus is formally approved in Swedish. This is a translation.

Learning outcomes

On completion of the course, participants shall be able to:

Knowledge and understanding

- Describe various techniques for Monte Carlo simulations of naturally stochastic processes, such as scattering processes.
- Describe various techniques for Monte Carlo and molecular dynamics calculations of equilibrium properties of complex systems with many degrees of freedom.

Skills and abilities

- Conduct Monte Carlo simulations of naturally stochastic processes.
- Conduct Monte Carlo and molecular dynamics simulations of equilibrium properties of complex systems.

Judgement and approach

- Recognise problems that can be approached with Monte Carlo or molecular dynamics methods.
- Explain the different sources of errors in numerical simulations and how the choice of algorithm may influence the convergence of simulations.

Course content

The course begins with a brief introduction to methods for Monte Carlo and molecular dynamics simulations. The student then performs six different simulation projects. The first five projects are predetermined and from different subject areas (e.g., astronomy, computational biology, theoretical chemistry, particle physics and medical radiation physics). The subject for the sixth and last project is chosen by the student in consultation with the course leader.

Teaching

The course is taught by lectures and supervised projects.

Assessment

Assessment is based on completion of written reports of the first five projects and an oral presentation of the final project.

Grading scale

Possible grades are Pass and Fail. To pass the course, the student must complete all the six project reports.

Language of instruction

The course is given in English.

Entry requirements

Basic competence in programming.

Additional information

None.