MH2102 Computational Physics 7.5 credits

Fysikaliska beräkningar på högprestandadatorer

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

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

Establishment

Course syllabus for MH2102 valid from Autumn 2007

Grading scale

A, B, C, D, E, FX, F

Education cycle

Second cycle

Main field of study

Specific prerequisites

Elementary statistical and solid-state physics. Elementary knowledge of programming and numerical methods.

Language of instruction

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

Intended learning outcomes

The goals of the course are to

- introduce the basic concepts and techniques of molecular dynamics and other methods of computer simulation of condensed matter,
- present and discuss the role of simulation as an independent method of research in condensed matter physics,
- demonstrate some results obtained by computer simulation which constitute an integral part of the modern condensed matter physics,

so that the students will be able to

- use and understand molecular dynamics simulation.

Course contents

Numerical methods in theoretical physics; the nature of mathematical experiments. Elements of statistical mechanics. Statistical ensembles and ergodic aspects. Comparative review of molecular dynamics algorithms. Description of macroscopic properties using collective variables and correlation functions. Using simulation for interpreting laboratory experiments (inelastic neutron scattering, etc). Statistical accuracy and systematic errors. Simulation of various phases of condensed matter: crystalline solids, liquids, glasses and quasi crystals. Constrained methods. Non-Newtonian algoritms of molecular dynamics. High-performance methods of simulation. Using parallel processing. Survey of Monte-Carlo methods. Methods of structural characterization using reversed Monte-Carlo. Quantum simulation.

Course literature

To be announced at course start.

Examination

- PRO1 - Project, 7.5 credits, grading scale: A, B, C, D, E, FX, F

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.

Other requirements for final grade

Project with examination (PRO1; 7,5 cr.).

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.