



SI2530 Computational Physics

7.5 credits

Beräkningsfysik

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 SI2530 valid from Autumn 2007

Grading scale

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

Education cycle

Second cycle

Main field of study

Engineering Physics, Physics

Language of instruction

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

Intended learning outcomes

To give an introduction to computational physics, which is a third area of physics beside experimental and theoretical physics. The goal is that the students should be able to:

- To understand the difference between simulations and other approximative and analytical methods
- To perform simulations and computations with available programs.
- Be able to write simple programs and make modifications of available programs.
- To understand the importance and limitations of a number of basic models with very broad applicability
- Be able to critically judge published results taking into account the limitations of the models and the statistical nature of several of the methods.

Course contents

The Monte Carlo and molecular dynamics methods. Simulations in different statistical mechanical ensembles. Computation of free energies. Stochastic dynamics. Applications to spin systems, fluids, polymers and biological macromolecules.

Specific prerequisites

Recommended prerequisites: Statistical mechanics and quantum mechanics corresponding to SI1161 quantum physics and some familiarity with computers and computer programming.

Course literature

M.P. Allen and D.J. Tildesley, Computer simulations of liquids and own material which is available at the web-page

Examination

- INL1 - Assignment, 4.5 credits, grading scale: A, B, C, D, E, FX, F
- LAB1 - Laboratory Work, 3.0 credits, grading scale: P, 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

Computer assignments (LAB1; 3 university credits)

Written exercises (INL1; 4,5 university credits).

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.