FSI3080 Computational Physics 7.5 credits

Beräkningsfysik

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

Establishment

Course syllabus for FSI3080 valid from Spring 2019

Grading scale

P, F

Education cycle

Third cycle

Specific prerequisites

Statistical mechanics and quantum mechanics, quantum physics, and some familiarity with computers and computer programming.

Language of instruction

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

Intended learning outcomes

After completed course, the PhD student should be able to:

- identify the difference between simulations and other approximative and analytical methods.
- perform simulations and computations with available programs.
- write simple programs and make modifications of available programs.
- describe the importance and limitations of a number of basic models with very broad applicability.
- 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.

Course literature

M.P. Allen and D.J. Tildesley, Computer simulations of liquids compiled with own material.

Examination

- LAB1 - Computer lab, 3.5 credits, grading scale: P, F
- INL1 - Assignment, 4.0 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.

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

Other requirements for final grade

Computer assignments. Written exercises.

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.