Computational Physics

Programme course

6 credits

Beräkningsfysik

TFYA53

Valid from: 2017 Spring semester

Determined by
Board of Studies for Electrical Engineering,
Physics and Mathematics

Date determined
2017-01-25

Main field of study

Applied Physics, Physics

Course level

Second cycle

Advancement level

A1X

Course offered for

- Physics and Nanoscience, Master's programme
- Materials Science and Nanotechnology, Master's programme

Specific information

Overlap with TFYA50

Entry requirements

Note: Admission requirements for non-programme students usually also include admission requirements for the programme and threshold requirements for progression within the programme, or corresponding.

Prerequisites

Statistical Mechanics, Solid State Physics, Condensed Matter Physics, Quantum Mechanics, Introductory Materials Science, computer and programming literacy. The emphasis is on general algorithms, so no specific programming language is required.

Intended learning outcomes

The course serves as an introduction to modern computational methods currently used in solid state physics, chemistry, biology and materials science. The main objective of the course is to present the principles underlying classical and ab-initio Monte Carlo and

Molecular Dynamics simulations. These methods are nowadays used extensively in the quest for new, man-made materials, in a wide range of industrial sectors (biotechnology, automotive, semiconductors, coatings).

Course content

The course is concerned with the theory and application of computer simulation of many-body systems. Following a review of the principles of statistical mechanics underlying computer simulations, the Monte Carlo (MC) and Molecular Dynamics (MD) techniques are introduced. Topics discussed include Monte Carlo integration, importance sampling, the Metropolis method, integration of equations of motion for many-body systems in MD, the Verlet algorithm and force calculation. MC and MD in various statistical ensembles, as well as analysis and visualisation techniques are also presented, with emphasis on their application to practical solutions of materials related problems.

Teaching and working methods

Lectures & Computer Laborations

Examination

UPG1	Written assignement	U, 3, 4, 5	4 credits
LAB1	Laboratory work	U, G	2 credits

Grades

Four-grade scale, LiU, U, 3, 4, 5

Department

Institutionen för fysik, kemi och biologi

Director of Studies or equivalent

Magnus Johansson

Examiner

Valeriu Chirita

Course website and other links

http://www.ifm.liu.se/undergrad/fysikgtu/coursepage.html?selection=all&sort=kk

Education components

Preliminary scheduled hours: 96 h
Recommended self-study hours: 64 h

Course literature

Additional literature

Books

M.P. Allen & D. J. Tildesley, *Computer Simulation of Liquids* Oxford Science Publications
ISBN: ISBN 0-19-855645-4

Common rules

Regulations (apply to LiU in its entirety)

The university is a government agency whose operations are regulated by legislation and ordinances, which include the Higher Education Act and the Higher Education Ordinance. In addition to legislation and ordinances, operations are subject to several policy documents. The Linköping University rule book collects currently valid decisions of a regulatory nature taken by the university board, the vice-chancellor and faculty/department boards.

LiU's rule book for education at first-cycle and second-cycle levels is available at http://styrdokument.liu.se/Regelsamling/Innehall/Utbildning_pa_grund-_och_avancerad_niva.