Project course in Computational Physics CDIO

Programme course

12 credits

Projektkurs i fysik, beräkningsfysik, CDIO

TFYA50

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

- Applied Physics and Electrical Engineering, M Sc in Engineering
- Materials Science and Nanotechnology, Master's programme
- Applied Physics and Electrical Engineering - International, M Sc in Engineering

Specific information

The Entrepreneurship part overlap with other CDIO courses and cannot be included more than once in a degree.

Exchange students may apply for the course after arrival to LiTH but before it starts. The international officer for exchange studies must be contacted before applying.

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, Materials Science, Solid programming knowledge.

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). A purpose for the course is also for the students to acquire knowledge and abilities within the general area of entrepreneurship, with particular focus on business planning for new ventures. After the course, students should be able to:

- account for models that describe what it takes for a new venture to have a stable basis for further development and to asess the level of development of ventures using such models; and
- account for the information and analyses needed to evaluate a development project from a business point of view and have the ability to collect and analyse relevant information for the purpose.

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 the application for practical solutions of materials related problems.

Teaching and working methods

The course follows the "Conceive Design Interact Operate (CDIO)" program at LiU and will use the project model "Linkoping Interactive Project Steering (LIPS)". Following a theoretical introduction to the computational methods, students will have to successfully complete a project related to materials science/thin films problems.

The course runs over the entire autumn semester.

Examination

UPG1	Entrepreneurship assignements	3 credits	U, G
LAB1	Laboratory work	2 credits	U, G
PRA1	Group working report followed by questions session.	7 credits	U, G

Grades are given as 'Fail' or 'Pass'.

Grades

Two-grade scale, U, G

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: 192 h
Recommended self-study hours: 128 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

Compendia

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.