

Computational Physics

Programme course

6 credits

Beräkningsfysik

TFYA90

Valid from: 2019 Spring semester

Determined by

Board of Studies for Electrical
Engineering, Physics and Mathematics

Date determined

2018-08-31

Main field of study

Applied Physics, Physics

Course level

Second cycle

Advancement level

A1X

Course offered for

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

Specific information

Some 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

Thermodynamics and statistical mechanics (TFYA12) and Quantum Mechanics (TFFY54), or corresponding courses that cover the same material and prerequisites. Also, basic understanding of computers and computer programming.

Intended learning outcomes

The course is an introduction to modern computational methods currently used in physics, materials science, quantum chemistry, and biology. The course covers the principles underlying both classical and quantum mechanical simulations, the core components of computational software, and practical examples. Included are classical and ab-initio Monte Carlo and Molecular Dynamics, variational calculus, many-particle quantum mechanics, and density functional theory (DFT). These methods are used extensively in fundamental research and for more applied tasks, e.g., the simulation of crystal growth, the design of new pharmaceuticals, and biotechnology, in both academia and industry. After completion of the course the student will be able to:

- Master the basic concepts and theories in computational physics based both on classical and quantum mechanical methods.
- Understand the main components of computer programs used for simulating matter systems and for finding numerical solutions to many-particle problems in quantum mechanics.
- Run computer software to predict properties of materials and molecular systems.

Course content

The course is about the theory and application of computer simulation of both classical and quantum mechanical 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 MC integration, importance sampling, the Metropolis method, integration of equations of motion for many-body systems in MD, the Verlet algorithm, and MC and MD in various statistical ensembles. An introduction to calculus of variations and many-particle quantum mechanics is given, and then Hartree, Hartree-Fock, and Density Functional Theory methods are derived and discussed, as well as, ab-initio Molecular Dynamics. The course covers the underlying theoretical concepts of these topics, an overview of how they are implemented in computational software, and some examples of how the methods are used. The course has four computer laborations with hands-on exercises for working with this type of computational software; generating data, analyzing, and visualizing the results.

Teaching and working methods

Theory part (22 h) and computer laborations (4x4 h)

Examination

| | | | |
|------|---------------------|-----------|------------|
| UPG1 | Written Assignments | 4 credits | U, 3, 4, 5 |
| LAB1 | Laboratory Work | 2 credits | U, G |

Grades

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

Department

Institutionen för fysik, kemi och biologi

Director of Studies or equivalent

Magnus Boman

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: 38 h

Recommended self-study hours: 122 h

Course literature

Books

M.P. Allen & D. J. Tildesley, *Computer Simulation of Liquids* Oxford Science Publications

ISBN: ISBN 0-19-855645-4

Compendia

Irina Yakymenko, Lecture notes on Computational Physics for Quantum Mechanical Many-Particle Systems

Common rules

Course syllabus

A syllabus has been established for each course. The syllabus specifies the aim and contents of the course, and the prior knowledge that a student must have in order to be able to benefit from the course.

Timetabling

Courses are timetabled after a decision has been made for this course concerning its assignment to a timetable module. A central timetable is not drawn up for courses with fewer than five participants. Most project courses do not have a central timetable.

Interrupting a course

The vice-chancellor's decision concerning regulations for registration, deregistration and reporting results (Dnr LiU-2015-01241) states that interruptions in study are to be recorded in Ladok. Thus, all students who do not participate in a course for which they have registered must record the interruption, such that the registration on the course can be removed. Deregistration from a course is carried out using a web-based form: www.lith.liu.se/for-studenter/kurskomplettering?l=sv.

Cancelled courses

Courses with few participants (fewer than 10) may be cancelled or organised in a manner that differs from that stated in the course syllabus. The board of studies is to deliberate and decide whether a course is to be cancelled or changed from the course syllabus.

Regulations relating to examinations and examiners

Details are given in a decision in the university's rule book:
<http://styrdokument.liu.se/Regelsamling/VisaBeslut/622678>.

Forms of examination

Examination

Written and oral examinations are held at least three times a year: once immediately after the end of the course, once in August, and once (usually) in one of the re-examination periods. Examinations held at other times are to follow a decision of the board of studies.

Principles for examination scheduling for courses that follow the study periods:

- courses given in VT1 are examined for the first time in March, with re-

examination in June and August

- courses given in VT2 are examined for the first time in May, with re-examination in August and October
- courses given in HT1 are examined for the first time in October, with re-examination in January and August
- courses given in HT2 are examined for the first time in January, with re-examination at Easter and in August.

The examination schedule is based on the structure of timetable modules, but there may be deviations from this, mainly in the case of courses that are studied and examined for several programmes and in lower grades (i.e. 1 and 2).

- Examinations for courses that the board of studies has decided are to be held in alternate years are held only three times during the year in which the course is given.
- Examinations for courses that are cancelled or rescheduled such that they are not given in one or several years are held three times during the year that immediately follows the course, with examination scheduling that corresponds to the scheduling that was in force before the course was cancelled or rescheduled.
- If teaching is no longer given for a course, three examination occurrences are held during the immediately subsequent year, while examinations are at the same time held for any replacement course that is given, or alternatively in association with other re-examination opportunities. Furthermore, an examination is held on one further occasion during the next subsequent year, unless the board of studies determines otherwise.
- If a course is given during several periods of the year (for programmes, or on different occasions for different programmes) the board or boards of studies determine together the scheduling and frequency of re-examination occasions.

Registration for examination

In order to take an examination, a student must register in advance at the Student Portal during the registration period, which opens 30 days before the date of the examination and closes 10 days before it. Candidates are informed of the location of the examination by email, four days in advance. Students who have not registered for an examination run the risk of being refused admittance to the examination, if space is not available.

Symbols used in the examination registration system:

** denotes that the examination is being given for the penultimate time.

* denotes that the examination is being given for the last time.

Code of conduct for students during examinations

Details are given in a decision in the university's rule book:
<http://styrdokument.liu.se/Regelsamling/VisaBeslut/622682>.

Retakes for higher grade

Students at the Institute of Technology at LiU have the right to retake written examinations and computer-based examinations in an attempt to achieve a higher grade. This is valid for all examination components with code "TEN" and "DAT". The same right may not be exercised for other examination components, unless otherwise specified in the course syllabus.

Retakes of other forms of examination

Regulations concerning retakes of other forms of examination than written examinations and computer-based examinations are given in the LiU regulations for examinations and examiners,

<http://stydokument.liu.se/Regelsamling/VisaBeslut/622678>.

Plagiarism

For examinations that involve the writing of reports, in cases in which it can be assumed that the student has had access to other sources (such as during project work, writing essays, etc.), the material submitted must be prepared in accordance with principles for acceptable practice when referring to sources (references or quotations for which the source is specified) when the text, images, ideas, data, etc. of other people are used. It is also to be made clear whether the author has reused his or her own text, images, ideas, data, etc. from previous examinations.

A failure to specify such sources may be regarded as attempted deception during examination.

Attempts to cheat

In the event of a suspected attempt by a student to cheat during an examination, or when study performance is to be assessed as specified in Chapter 10 of the Higher Education Ordinance, the examiner is to report this to the disciplinary board of the university. Possible consequences for the student are suspension from study and a formal warning. More information is available at <https://www.student.liu.se/studenttjanster/lagar-regler-rattigheter?l=sv>.

Grades

The grades that are preferably to be used are Fail (U), Pass (3), Pass not with distinction (4) and Pass with distinction (5). Courses under the auspices of the faculty board of the Faculty of Science and Engineering (Institute of Technology) are to be given special attention in this regard.

1. Grades U, 3, 4, 5 are to be awarded for courses that have written examinations.
2. Grades Fail (U) and Pass (G) may be awarded for courses with a large degree of practical components such as laboratory work, project work and group work.

Examination components

1. Grades U, 3, 4, 5 are to be awarded for written examinations (TEN).
2. Grades Fail (U) and Pass (G) are to be used for undergraduate projects and other independent work.

3. Examination components for which the grades Fail (U) and Pass (G) may be awarded are laboratory work (LAB), project work (PRA), preparatory written examination (KTR), oral examination (MUN), computer-based examination (DAT), home assignment (HEM), and assignment (UPG).
4. Students receive grades either Fail (U) or Pass (G) for other examination components in which the examination criteria are satisfied principally through active attendance such as other examination (ANN), tutorial group (BAS) or examination item (MOM).

The examination results for a student are reported at the relevant department.

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.