

Computational Physics

Programme course

6 credits

Beräkningsfysik

TFYA90

Valid from: 2021 Spring semester

Determined by

Board of Studies for Electrical Engineering,
Physics and Mathematics

Date determined

2020-09-29

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
- Master of Science in Applied Physics and Electrical Engineering - International
- Master of Science in Applied Physics and Electrical Engineering
- Master's Programme in Materials Physics for Nano and Quantum Technology

Specific information

Some overlap with TFYA50

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

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

Grades

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

Department

Institutionen för fysik, kemi och biologi

Director of Studies or equivalent

Magnus Boman

Examiner

Davide Sangiovanni

Course website and other links

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

Education components

Preliminär schemalagd tid: 38 h

Rekommenderad självstudietid: 122 h

Course literature

Böcker

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

Kompendier

Iryna Yakymenko, Lecture Notes on Quantum Dynamics

Common rules

Course syllabus

A syllabus must be 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.

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: <https://www.lith.liu.se/for-studenter/kurskomplettering?f=en>.

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 Dean is to deliberate and decide whether a course is to be cancelled or changed from the course syllabus.

Guidelines relating to examinations and examiners

For details, see Guidelines for education and examination for first-cycle and second-cycle education at Linköping University, Dnr LiU-2019-00920 (<http://styrdokument.liu.se/Regelsamling/VisaBeslut/917592>).

An examiner must be employed as a teacher at LiU according to the LiU Regulations for Appointments, Dnr LiU-2017-03931

(<https://styrdokument.liu.se/Regelsamling/VisaBeslut/622784>). For courses in second-cycle, the following teachers can be appointed as examiner: Professor (including Adjunct and Visiting Professor), Associate Professor (including Adjunct), Senior Lecturer (including Adjunct and Visiting Senior Lecturer), Research Fellow, or Postdoc. For courses in first-cycle, Assistant Lecturer (including Adjunct and Visiting Assistant Lecturer) can also be appointed as examiner in addition to those listed for second-cycle courses. In exceptional cases, a Part-time Lecturer can also be appointed as an examiner at both first- and second cycle, see Delegation of authority for the Board of Faculty of Science and Engineering.

Forms of examination

Principles for examination

Written and oral examinations and digital and computer-based 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 in March 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 three times during the school year in which the course is given according to the principles stated above.

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.

When a course is given for the last time, the regular examination and two re-examinations will be offered. Thereafter, examinations are phased out by offering three examinations during the following academic year at the same times as the examinations in any substitute course. If there is no substitute course, three examinations will be offered during re-examination periods during the following academic year. Other examination times are decided by the board of studies. In all cases above, the examination is also offered one more time during the academic year after the following, unless the board of studies decides 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.

Retakes of other forms of examination

Regulations concerning retakes of other forms of examination than written examinations and digital and computer-based examinations are given in the LiU guidelines for examinations and examiners, <http://styrdokument.liu.se/Regelsamling/VisaBeslut/917592>.

Registration for examination

Until January 31 2021, the following applies according to previous guidelines: In order to take an written, digital or computer-based examination 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.

From February 1 2021, new guidelines applies for registration for written, digital or computer-based examination, Dnr LiU-2020-02033 (<https://styrdokument.liu.se/Regelsamling/VisaBeslut/622682>).

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 digital and computer-based examinations in an attempt to achieve a higher grade. This is valid for all examination components with code "TEN", "DIT" and "DAT". The same right may not be exercised for other examination components, unless otherwise specified in the course syllabus.

A retake is not possible on courses that are included in an issued degree diploma.

Grades

The grades that are preferably to be used are Fail (U), Pass (3), Pass not without distinction (4) and Pass with distinction (5).

- Grades U, 3, 4, 5 are to be awarded for courses that have written or digital examinations.
- 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.
- Grades Fail (U) and Pass (G) are to be used for degree projects and other independent work.

Examination components

The following examination components and associated module codes are used at the Faculty of Science and Engineering:

- Grades U, 3, 4, 5 are to be awarded for written examinations (TEN) and digital examinations (DIT).
- 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), digital preparatory written examination (DIK),

oral examination (MUN), computer-based examination (DAT), home assignment (HEM), and assignment (UPG).

- 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 tutorial group (BAS) or examination item (MOM).
- Grades Fail (U) and Pass (G) are to be used for the examination components Opposition (OPPO) and Attendance at thesis presentation (AUSK) (i.e. part of the degree project).

In general, the following applies:

- Mandatory course components must be scored and given a module code.
- Examination components that are not scored, cannot be mandatory. Hence, it is voluntary to participate in these examinations, and the voluntariness must be clearly stated. Additionally, if there are any associated conditions to the examination component, these must be clearly stated as well.
- For courses with more than one examination component with grades U,3,4,5, it shall be clearly stated how the final grade is weighted.

For mandatory components, the following applies: If special circumstances prevail, and if it is possible with consideration of the nature of the compulsory component, the examiner may decide to replace the compulsory component with another equivalent component. (In accordance with the LiU Guidelines for education and examination for first-cycle and second-cycle education at Linköping University, <http://styrdokument.liu.se/Regelsamling/VisaBeslut/917592>).

For written examinations, the following applies: If the LiU coordinator for students with disabilities has granted a student the right to an adapted examination for a written examination in an examination hall, the student has the right to it. If the coordinator has instead recommended for the student an adapted examination or alternative form of examination, the examiner may grant this if the examiner assesses that it is possible, based on consideration of the course objectives. (In accordance with the LiU Guidelines for education and examination for first-cycle and second-cycle education at Linköping University, <http://styrdokument.liu.se/Regelsamling/VisaBeslut/917592>).

Reporting of examination results

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

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, such as degree projects, project reports, etc. (this is sometimes known as “self-plagiarism”).

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=en>.

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://stydokument.liu.se/Regelsamling/Innehall/Utbildning_pa_grund-_och_avancerad_niva.