

# Project course in Computational Physics CDIO

Programme course

12 credits

Projektkurs i fysik, beräkningsfysik, CDIO

TFYA50

Valid from: 2018 Spring semester

**Determined by**

Board of Studies for Electrical  
Engineering, Physics and Mathematics

**Date determined**

## Main field of study

Applied Physics, Physics

## Course level

Second cycle

## Advancement level

A1X

## Course offered for

- Materials Science and Nanotechnology, Master's Programme
- Applied Physics and Electrical Engineering, M Sc in Engineering
- 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 Faculty coordinators 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 assess 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 "Linköping 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 assignments	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, older version, U, G

## 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: 192 h

Recommended self-study hours: 128 h

## Course literature

### Books

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

ISBN: ISBN 0 - 19 - 855645 - 4

### Compendia

## 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](http://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 without 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](http://styrdokument.liu.se/Regelsamling/Innehall/Utbildning_pa_grund-_och_avancerad_niva).