Computational Physics, 6 credits (TFYA90) HT2 2020

Beräkningsfysik, 6 hp

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-inito 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-intio 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	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 Boman

Examiner

Davide G. Sangiovanni (physics building, entrance 57, office G408)
davide.sangiovanni@liu.se

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

Compendiums

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