



Faculty of Technology and Science
Physics

Syllabus

Course Approval

The syllabus was approved by the Faculty Board of Technology and Science on 26 November 2008 , and is valid from the Spring semester of 2008 at Karlstad University.

Course Code: CBAD82

Computational Physics, 7.5 ECTS Credits
(Beräkningsfysik, 7.5 Swedish credit points)

Degree Level: Master

Progressive Specialisation: A1F (Second cycle, has second-cycle course/s as entry requirements)

Language of Instruction

The language of instruction is English but the course can also be taught in Swedish if all students speak Swedish.

Prerequisites

To be accepted to the course, approval on the following courses (or the equivalent) is required: Quantum Physics I and II, Physics: Solid State Physics, and Basic Mathematical Physics.

Major Field of Study

FYA (Physics)

Learning Outcomes

Upon completion of the course, students should be able to:

- use numerical methods to model physical systems on different length- and time scales
- critically select different numerical methods to solve different types of physical and technical problems
- implement numerical algorithms into MATLAB and visualize the results of the computations
- describe the basis of FEM and use it to solve partial differential equations
- describe the basis of stochastic simulation methods such as the Monte Carlo method and use them
- describe and use molecular dynamic simulation
- use the variation method to solve quantum mechanical problems
- describe different methods to compute the electron structure of solid materials.

Content and Form of Instruction

The course introduces important numerical physical computation methods in three main fields: continuum methods, stochastic methods, and quantum mechanical methods. Numerical computations are implemented in MATLAB and in routines from C- and Fortran libraries.

Course content:

- The basics of the finite element method (FEM). Using FEM to solve problems related to the strength of materials.
- The solution to the Schrödinger equation using the variation method. Computation of the electron structure of crystalline materials: introduction to the Hartree-Fock method and density functional theory (DFT).

- Simulations using molecular dynamics, introduction to quantum-molecular dynamics. The Monte Carlo method.
- Parallelization and high-performance computations.

Reading List

See separate document.

Examination

Examination is in the form of solutions to the obligatory implementation assignments, which are presented in written and oral form, and written and oral presentation of a specialized study. Participation in the presentation seminars is required to pass the course.

Grades

One of the grades 5 (Distinction), 4 (Some Distinction), 3 Pass , or Fail (U), is awarded in the examination of the course.

Quality Assurance

Follow-up relating to learning conditions and goal-fulfilment takes place both during and upon completion of the course in order to ensure continuous improvement. Course assessment is based on student views and experiences as reported in written course evaluations and/or group discussions. Students will be informed of the result of the evaluation and of the measures to be taken.

Course Certificate

A course certificate will be provided upon request.

Additional Information

Students who enrolled before 1 July 2007 will complete their studies in accordance with the requirements of the earlier admission. Upon completion students may request degree and course certificates to be issued under the current ordinance if they meet its requirements.

The local regulations for studies at the Bachelor's and Master's levels at Karlstad University stipulate the obligations and rights of students and staff.

The course is a mandatory part of the program in Engineering Physics and the Master program in Nanomaterials.

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