Reg No: CBAD82/20241

Faculty of Health, Science and Technology
Physics

Syllabus

Computational Physics

Course Code:	CBAD82
Course Title:	Computational Physics *Beräkningsfysik*
Credits:	7.5
Degree Level:	Master's level
Progressive Specialisation:	Second cycle, has second-cycle course/s as entry requirements (A1F)

Major Field of Study:
FYA (Physics)
TKA (Engineering Physics)

Course Approval
The syllabus was approved by the Faculty of Health, Science and Technology 2023-09-04, and is valid from the Spring semester 2024 at Karlstad University.

Prerequisites
Numerical Methods (7.5 ECTS credits), Mathematical Physics II (7.5 ECTS credits), Solid State Physics (7.5 ECTS credits), and registered for Quantum Physics II (7.5 ECTS credits), and upper secondary level English 6, or equivalent

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 various types of physical and technical problems,
- implement numerical algorithms and visualise the results of the computations,
- describe the basis of electronic structure theory,
- use the variation method to solve quantum mechanical problems,

- describe different methods to compute the electron structure of solid materials,
- use existing electronic structure program package for calculating spectroscopic properties,
- describe the basis of stochastic simulation methods such as the Monte Carlo method and use them, and
- describe and use molecular dynamic simulation.

Content
The course introduces important numerical physical computation methods in different fields. The numerical simulations are implemented in a suitable programming language (for instance Fortran, C, MATLAB, Python) or carried out in specific simulation software.

Course content:
The basics of electronic structure theory and calculation methods.
The solution to the Schrödinger equation using the variation method. Computation of the electronic 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.
Parallelisation and high-performance computations.

Reading List
See separate document.

Examination
Assessment is in the form of solutions to the mandatory assignments, which are presented in written and oral form, and written and oral presentation of an individual independent study project. Participation in the presentation seminars is required for course completion.

If students have a decision from Karlstad University entitling them to Targeted Study Support due to a documented disability, the examiner has the right to give such students an adapted examination or to examine them in a different manner.

Grades
One of the grades Distinction (VG), Pass (G), or Fail (U) is awarded in the examination of the course. For students in Engineering, one of the grades 5 (Pass with Distinction), 4 (Pass with Some Distinction), 3 (Pass), or U (Fail) 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 evaluation is partly based on student views and experiences obtained in accordance with current regulations and partly on other data and documentation. Students will be informed of the result of the evaluation and of any measures to be taken.

Course Certificate
A course certificate will be provided upon request.

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

Required course for the Master of Science programme in Engineering Physics and the

preparatory programme for a Master of Science in Engineering Physics.