



Faculty of Science

BERM06, Applied Computational Science - Chemistry: Master's Degree Project, 30 credits

*Tillämpad beräkningsvetenskap - Kemi: Examensarbete för masterexamen, 30
högskolepoäng*
Second Cycle / Avancerad nivå

Details of approval

The syllabus was approved by Study programmes board, Faculty of Science on 2023-12-07. The syllabus comes into effect 2023-12-07 and is valid from the autumn semester 2024.

General information

The course is a compulsory course for second-cycle studies for a Degree of Master of Science (120cr) in Applied Computational Science with specialisation in Chemistry.

Language of instruction: English

Main field of study

Specialisation

Applied Computational
Science

A2E, Second cycle, contains degree project for Master of
Arts/Master of Science (120 credits)

Learning outcomes

The aim of the degree project is that the student shows knowledge understanding, competence, skills, ability, judgement and approach in accordance with the requirements for obtaining a Degree of Master of Science in Applied Computational Science with specialisation in Chemistry through an independent project. The degree project shall be specialised and show that the student can apply computational methodology within computational and natural sciences.

Knowledge and understanding

After completing the course the student shall be able to independently:

- in detail describe and use methods within a specialisation of some sub-field of Chemistry and be able to discuss the possibilities and limitations of these methods independently,

- describe research questions in a sub-field of Chemistry.

Competence and skills

After completing the course the student should be able to:

- critically and independently analyse, manage and formulate questions that are relevant to research or development work in a sub-field of Chemistry,
- independently plan and execute a scientific project work within given time frames using appropriate computational methods,
- give a clear and thorough written report on the results of the completed project work and the knowledge and arguments on which they are based,
- at an oral presentation summarize the most important results of the project work as well as briefly discuss the knowledge and arguments that underlie them,
- summarize the most important results of the completed project work in a written popular scientific report.

Judgement and approach

After completing the course the student should be able to independently:

- discuss relevant scientific, societal and ethical aspects related to the completed project work,
- take responsibility for their knowledge development, thereby identifying their own need for further knowledge and planning to acquire the needed knowledge.

Course content

The content and execution of the degree project are planned in consultation with a supervisor. The degree project consists of an independent smaller research or development assignment that includes the application of computational methods to a problem in the natural sciences in a broad sense. The degree project should relate to current projects at the faculty of science or to problems within the subject area at companies or other institutions within or outside the university. If the work is carried out outside of the faculty of science, there should also be a supervisor from the faculty of science with competence in computational science.

Course design

The thesis requires a literature review and special studies. In addition, there are a number of compulsory activities in the form of lectures and seminars which treat scientific, academic, and popular science communication, including both written and oral presentation, discussion and feedback.

The project work corresponds to twenty weeks of full-time studies. During the project, guidance is given by a qualified supervisor. If the work is carried out under supervision outside the department, another supervisor is appointed at the department.

At the start of the course, the student, in consultation with the supervisor, establishes a study plan containing a description of the assignment, a problem analysis and a project timeline.

During the project, progress is reported in form of a half-time report and a presentation in a midterm seminar (15cr).

Finally, the work is presented in the form of a project report in English with a popular scientific description in Swedish or English. The work is also presented orally at a public seminar for discussion, criticism and analysis (15cr). Prior to the presentation, the student, together with their supervisor, must review their work based on the learning objectives in this syllabus and / or in the goals of the Higher Education Act for the master's degree.

Assessment

Examination is based on:

- a written half-time report and an oral presentation of the project work at the midterm seminar (15cr),
- a written scientific report, a brief written popular scientific summary, and an oral presentation at the end during the defense of the final report (15cr).

In addition, an approved written timetable established at the beginning of the work, participation in all compulsory activities, and a brief reflection on the student's own learning are required.

The written report must be submitted to the examiner in a version that permits examination at least two weeks before the seminar. The department is responsible for the multiplication of the report according to the requirements of the university and the faculty. Upon final approval, the student is responsible for archiving the report in a system supplied by the university.

The examiner, in consultation with Disability Support Services, may deviate from the regular form of examination in order to provide a permanently disabled student with a form of examination equivalent to that of a student without a disability.

Grades

Grading scale includes the grades: Fail, Pass, Pass with distinction

To obtain the grade **pass**, the following examination parts are required:

- a timetable and project description established at the beginning of the work,
- participation in all compulsory elements,
- an oral presentation of the project as part of the midterm seminar and halftime seminar,
- a scientific written report on the work,
- an oral presentation of the work,
- a written popular scientific description of the work,
- a brief reflection on the student's own learning.

The final grade is determined by summarizing the results of these parts where the largest weight is given to the report. The examiner decides the grade in consultation with the supervisor. If the examiner assesses that the degree project can not be approved, the student shall be given the possibility to supplement the work for a renewed assessment within approximately half a semester. If the work does not meet the learning outcomes of the course after this renewed assessment, the examiner may decide to fail it.

To obtain the grade **pass with distinction**, the work may not exceed the time plan by more than 20%.

Entry requirements

Admission to the course requires courses corresponding to MATA04 Mathematics for Scientists 2, 15 credits, NUMA01 Computational Programming in Python, 7.5 credits, BERN01 Modelling in Computational Science, 7.5 credits, and BERN02 Reproducible Data Science and Statistical Learning, 7.5 credits. Furthermore, 15 credits in Chemistry at the advanced level are required, as well as knowledge corresponding to English 6/B.

Further information

The course is given at the Center for Mathematical Sciences, Lund University.