LUND UNIVERSITY

Faculty of Science

BERN01, Computational Science: Modelling in Computational Science, 7.5 credits

Beräkningsvetenskap: Modellering i beräkningsvetenskap, 7,5 högskolepoäng

Second Cycle / Avancerad nivå

Details of approval

The syllabus was approved by Study programmes board, Faculty of Science on 2022-12-09 to be valid from 2022-12-09, autumn semester 2023.

General Information

The course is a compulsory course in the second cycle for a degree of Master of Science in Computational Science and for a degree of Master of Science in Applied Computational Science. The course can be included as an optional course within a master's degree in Mathematics and it can also be given as an independent course.

Language of instruction: English

Main field of studies	*Depth of study relative to the degree requirements*
Mathematics with specialization in Numerical Analysis	A1N, Second cycle, has only first-cycle course/s as entry requirements
Applied Computational Science	A1N, Second cycle, has only first-cycle course/s as entry requirements
Computational Science	A1N, Second cycle, has only first-cycle course/s as entry requirements

Learning outcomes

The overall goal of the course is to give the students an overview of fundamental modelling techniques in computational science. The students get an introduction to mathematical modelling of problems in the sciences and to how these models can be treated using computational methods. In particular, differential equation based models, machine learning for databased models, and Monte-Carlo methods for statistical models, are discussed.

Knowledge and understanding

On completion of the course, students shall be able to:

- explain the difference between a mathematical model and a numerical method for solving this model,
- describe how differential equations can be used to implement models that offer solutions to problems from areas such as physics, biology and epidemiology,
- explain what a discretisation of a differential equation is,
- describe the basic theory of Monte Carlo methods,
- explain the Metropolis-Hastings algorithm and what a Markov chain is,
- explain the basic ideas of machine learning and how machine learning relates to regression analysis,
- describe different types of errors in computational modeling, such as modeling errors, discretisation errors and statistical errors.

Competence and skills

On completion of the course, students shall be able to:

- formulate mathematical models for scientific problems,
- deduce, implement and apply numerical methods to solve systems of ordinary differential equations (ODEs),
- construct Markov chain Monte Carlo (MCMC) algorithms for simulations of systems with many degrees of freedom, such as an Ising magnet or a Lennard-Jones fluid,
- estimate auto correlations and statistical errors from MCMC simulations,
- apply methods that improve the efficiency of MCMC calculations,
- implement machine learning algorithms to learn models from large data sets,
- estimate various types of errors in numerical calculations,
- plan, and with suitable methods conduct, qualified tasks within the scope of the course, and within a given time frame.

Judgement and approach

On completion of the course, students shall be able to:

- evaluate error sources in mathematical models and their numerical treatment,
- reflect upon the compromises made during the development of computational models and evaluate their eventual effects,
- critically evaluate the application of methods and interpret predictions obtained within a project,
- evaluate their own responsibility for how the acquired knowledge is used and discuss the possibilities of the course subject to contribute to sustainable societal development.

Course content

The course treats:

- Differential equation based modelling: Numerical methods to solve ODEs and convergence order. Applications to for instance predicting the spread of diseases and cell programming will be used.
- MCMC based modelling: Central Limit Theorem, Metropolis-Hasting algorithm and error propagation will be covered with examples from statistical thermodynamics.
- Machine learning and big data: We will cover the use of large data sets for

creating models by training machine learning algorithms and which conditions are needed to create such models. This will be carried out on climate science applications.
- Sources of errors in computational models, such as modeling errors, discretisations errors and statistical errors.
- Relevant aspects concerning the fields possibilities to contribute to sustainable social development.

Course design

The teaching consists of lectures. Three compulsory projects carried out in small groups are included in the course. Attendance at all oral group presentations of the project results is mandatory.

Assessment

The examination takes place in writing in the form of individual project reports and through oral presentations of the project in groups.

For students who have not passed the regular examination, an additional examination opportunity is offered in close connection with this.

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.

Subcourses that are part of this course can be found in an appendix at the end of this document.

Grades

Marking scale: Fail, Pass, Pass with distinction.
For a Pass grade on the whole course, the student must have Pass grades on the written project reports and oral group project presentations.

The grading scale for the oral project presentations is Fail, Pass, while the project reports are graded according to grading scale Fail, Pass, Pass with Distinction.

The grade Pass with distinction on the whole course is decided by the grade on the project reports.

Entry requirements

Either a Bachelor's Degree in Physics or at least 90 ECTS credits in natural sciences or engineering, including 43.5 credits in mathematics, of which a course corresponding to NUMA01 Numerical Analysis: Computational Programming with Python, 7.5 credits and 7.5 credits in basic Mathematical statistics. English course 6/B.

Subcourses in BERN01, Computational Science: Modelling in Computational Science

Applies from H23

2301 Written Project Reports, 4,5 hp
Grading scale: Fail, Pass, Pass with distinction

2302 Oral Presentations, 3,0 hp
Grading scale: Fail, Pass