Faculty of Science

BERN07, Computational Science: Uncertainty Quantification & Data-driven Modelling, 7.5 credits

Beräkningsvetenskap: Osäkerhetskvantifiering och datadriven modellering, 7,5 högskolepoäng

Second Cycle / Avancerad nivå

Details of approval

The syllabus was approved by Study programmes board, Faculty of Science on 2024-04-16. The syllabus comes into effect 2024-04-16 and is valid from the spring semester 2025.

General information

The course is an elective course in the second cycle for a degree of Master of Science in Computational Science, Applied Computational Science, or Mathematics. The course can also be given as an independent course.

Language of instruction: English

Main field of study	*Specialisation*
Mathematics with specialization in Numerical Analysis	A1F, Second cycle, has second-cycle course/s as entry requirements
Computational Science	A1F, Second cycle, has second-cycle course/s as entry requirements
Applied Computational Science	A1F, Second cycle, has second-cycle course/s as entry requirements

Learning outcomes

The overarching goal of the course is that the students on completion of the course should have acquired basic knowledge regarding numerical methods for uncertainty quantification and relevant data-driven modeling in computational science. This includes forward uncertainty propagation from inputs to responses, inverse parameter estimation through Bayesian approaches, surrogate modeling for accelerating multi-query simulations, and observational data integration into dynamical models.

Knowledge and understanding

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

- explain the critical significance of uncertainty quantification in computational science, as well as relevant important concepts
- identify the existence and propagation of uncertainties in computational modeling and analysis
- explain the mechanism of stochastic Galerkin and collocation methods, as well as their connections and differences
- describe the connections among estimators related to Bayesian inference
- explain Monte Carlo and importance sampling from the quadrature viewpoint
- explain the use of Galerkin projections in deterministic, stochastic, and model-reduction contexts
- explain the proper orthogonal decomposition and its error control
- describe the connections among Gaussian models introduced with Bayesian inference, Gaussian process regression, and Kalman filters

Competence and skills

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

- numerically solve elliptic PDEs with random parameters using stochastic spectral methods (forward problems)
- numerically infer system parameters via Bayesian techniques (inverse problems)
- use sampling methods to estimate characteristic outputs of interest (uncertainty propagation)
- construct data-driven surrogate models for multi-query simulations (acceleration)
- assimilate observational data into dynamical models using Kalman filters (data integration)

Judgement and approach

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

- evaluate uncertainty sources in computational models, data sets, and their numerical treatments
- critically reflect on the probabilistic methods and interpret their results for uncertainty quantification in scientific and engineering applications
- independently apply data-driven numerical methods in a project work

Course content

The course treats:

- Important concepts in uncertainty quantification (UQ), such as verification vs. validation, intrusive vs. non-intrusive, and forward vs. inverse UQ

- Numerical discretisation for PDEs with random parameters: stochastic Galerkin and stochastic collocation
- Bayesian inference and its applications to parameter estimation
- Sampling techniques: Monte Carlo and importance sampling
- Gaussian processes for surrogate modeling
- Basics of projection-based and data-driven model reduction
- Data assimilation with Kalman filters

Course design

The teaching consists of lectures and assignments. The assignments are not compulsory but preparatory for the oral exam.

Assessment

The examination consists of a written project report and an oral examination at the end of the course.

For students who have not passed the regular exam, an additional exam 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.

Grades

Grading scale includes the grades: Fail, Pass, Pass with distinction
The grading scale for the project report is Fail, Pass, while the oral examination is graded according to grading scale Fail, Pass, Pass with Distinction.

For a **Pass** grade on the whole course, the student must have **Pass** grades on the written project report and oral examination.

The grade **Pass with distinction** on the whole course is decided by the grade on the oral examination.

Entry requirements

Admission to the course requires English 6/b and at least 90 credits in natural sciences or engineering, of which at least 45 credits should be in mathematics and/or numerical analysis, including knowledge corresponding to the courses NUMA01 Computational Programming with Python, 7.5 credits, MASA02 Mathematical Statistic, Basic Course, 15 credits, and NUMN32 Numerical Methods for Differential Equations, 7.5 credits.

Further information

The course is offered by the Centre for Mathematical Sciences, Lund University.