DN2280 Computational Methods from Micro to Macro Scales 7.5 credits

Beräkningsmetoder från mikro- till makroskalor

This is a translation of the Swedish, legally binding, course syllabus.

Establishment

Course syllabus for DN2280 valid from Autumn 2009

Grading scale

A, B, C, D, E, FX, F

Education cycle

Second cycle

Main field of study

Specific prerequisites

Single course students: 90 university credits including 45 university credits in Mathematics or Information Technology. English B, or equivalent.

Language of instruction

The language of instruction is specified in the course offering information in the course catalogue.

Intended learning outcomes

After completing this master level course the student will be able to model, analyze and compute solutions to multi-scale model problems from Schrödingers equation, for nuclei-electron systems, over molecular dynamics to Euler and Navier-Stokes equation for continuum fluids.

Course contents

Differential equations are fundamental for the modeling in Science and Engineering. As the computational power increase, it becomes feasible to use more accurate differential equation models and solve more demanding problems: for instance to determine input data from fundamental principles and to optimally reconstruct input data using measurements.The course includes lectures, computer exercises and student presentations on models, analysis and computational methods from nuclei-electron micro-systems to Euler and Navier-Stokes macro-systems for continuum fluids, using a unified mathematical method to derive and explain the coupling between the models on the different scales.
- Relation between Schrödinger-molecular dynamics-continuum partial differential equations

- Ehrenfest dynamics and surface-hopping

- the Born-Oppenheimer approximation

- electron structure calculation methods

- bridging ab initio and empirical molecular dynamics

- molecular dynamics: thermodynamics and statistical mechanics

- molecular dynamics: ensembles and simulations

- stochastic Langevin and Smolchuwski molecular dynamics

- molecular dynamics reaction paths and rates

- Euler and Navier-Stokes macroscopic equation derived from microscopic molecular dynamics

- project presentations on applications.

Course literature

Lecture notes.

Examination

- TEN1 - Examination, 4.0 credits, grading scale: A, B, C, D, E, FX, F
- LAB1 - Laboratory, 3.5 credits, grading scale: P, F

Based on recommendation from KTH's coordinator for disabilities, the examiner will decide how to adapt an examination for students with documented disability.

The examiner may apply another examination format when re-examining individual students.

If the course is discontinued, students may request to be examined during the following two academic years.

In this course all the regulations of the code of honor at the School of Computer science and Communication apply, see: http://www.kth.se/csc/student/hederskodex/1.17237?l=en_UK.

Ethical approach

- All members of a group are responsible for the group's work.
- In any assessment, every student shall honestly disclose any help received and sources used.
- In an oral assessment, every student shall be able to present and answer questions about the entire assignment and solution.