FSF3564 Mathematical and Computational Methods from Micro to Macro Scales 7.5 credits

Matematiska och numeriska metoder från mikro- till makro-skalor

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

Establishment

Course syllabus for FSF3564 valid from Autumn 2015

Grading scale

G

Education cycle

Third cycle

Specific prerequisites

A Master degree including at least 30 university credits (hp) in in Mathematics (including differential equations and numerical analysis).

Language of instruction

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

Intended learning outcomes

Students will be able to use, relate and critically evaluate analytical and numerical approximations on different scales.

Course contents

The Schrödinger equation, which accurately models nuclei-electron system without unknown parameters, is the basis for condensed matter physics and computational chemistry. An important issue is its high computational complexity, e.g. already for a water molecule it means to solve a partial differential equation in 39 dimensions. Computational approximations are therefore needed and the goal of the course is to present, use and understand numerical methods for the important coarse-grained approximations.

The complexity is reduced by classical approximation of the nuclei, using Born-Oppenheimer dynamics. To computationally solve the quantum problem for the electrons the Hartree-Fock and Kohn-Sham density functional theory is important and leads to an ab initio molecular dynamics model. The ab initio molecular dynamics can be simplified by empirical potentials. Thermal fluctuations in an ensemble at constant temperature introduces stochastics into the dynamics which leads to the Langevin molecular dynamics, or variants thereof. On long time scales and in the high friction limit this dynamics can be described without the velocities by the Smoluchowski equation. The next step in the coarse-graining process is to derive partial differential equations for the mass, momentum and energy of a continuum fluid, which determines the otherwise unspecified stress tensor and heat flux.

Disposition

1. The Schrödinger equation

a. Introduction and postulates

b. Properties (conservation of **L_2**-norm, symmetries, relation with classical mechanics, etc.)

c. Numerical methods for the Schrödinger equation

d. Approximations

- The Born-Oppenheimer approximation
- The Hartree-Fock method
- Density functional theory

2. Molecular dynamics

a. Microcanonical and canonical ensembles

b. Car-Parrinello and Langevin molecular dynamics

c. Numerical methods for molecular dynamics

d. Reaction rates and reaction paths

e. Bridging ab initio and empirical methods

3. Continuum problems

a. Continuum fluid dynamics derived from molecular dynamics

b. A phase-field continuum model derived from Smoluchowski MD

Course literature

Cances E., Defranceschi M., Kutzelnigg W., LeBris C., Maday Y., Computational Chemistry: a primer, n Handbook of Numerical Analysis, X, North-Holland 2003. some pages.
Elliott H. Lieb and Robert Seiringer, The Stability of Matter in Quantum mechanics, Cambridge University Press 2010, chapter 2 and 3.
E Weinan, Principles of Multiscale Modeling, Cambridge University Press 2011.

Examination

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.

Homework problems

Computer assignments

Written exam

Other requirements for final grade

Homework and computer assignments completed
Written exam passed

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.