BB2540 Multiscale Modelling in Chemistry and Biology 10.0 credits

Flerskalig modellering i kemi och biologi

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

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

Establishment

Course syllabus for BB2540 valid from Spring 2012

Grading scale

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

Education cycle

Second cycle

Main field of study

Biotechnology

Language of instruction

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

Intended learning outcomes

After the course, you should be able to

- outline the purpose and functions of multi-scale modeling;
- give examples of different types of intermolecular interactions;
- describe the fundamental concepts and important approaches in relation to a modeling scale;
- choose an appropriate modeling tool for a given property of a molecular system, with respect to the modeling scale, and apply the modeling tool to calculate the property;
- combine modeling tools at different scales to model a complex biological phenomenon;
- explain how the modeling approaches at different scales interrelate.

Course contents

1. Introduction to Multi-scale modelling

2. Review of underlying electronic structure calculations

3. Modelling intermolecular interactions

4. Methods for atomistic scale simulations

5. Introduction to currently used molecular dynamics simulation softwares

6. Meso-scale simulation methods

7. Application of multi-scale modeling to protein structure and folding

8. Computer exercises

Specific prerequisites

At least 150 credits from grades 1, 2 and 3 of which at least 100 credits from years 1 and 2, and bachelor's work must be completed.
The 150 credits should include a minimum of 20 credits within the fields of Mathematics, Numerical Analysis and Computer Sciences, 5 credits of these must be within the fields of Numerical Analysis and Computer Sciences.

Course literature

Andrew R. Leach,“**Molecular Modeling, Principles and Applications”,** 2nd edition;

Lecture notes and handouts will be distributed after each lecture.

Examination

- LAB1 - Laboratory Work, 2.0 credits, grading scale: P, F
- PRO1 - Project 1, 1.5 credits, grading scale: A, B, C, D, E, FX, F
- PRO2 - Project 2, 1.5 credits, grading scale: A, B, C, D, E, FX, F
- TEN1 - Examination, 3.0 credits, grading scale: A, B, C, D, E, FX, F
- UPG1 - Home Assignment, 2.0 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.

Other requirements for final grade

To pass the course, you should

- attend the lectures and fulfill 10 course assignments (UPG1; 2 credits);
- fulfill 4 computational labs on multi-scale modeling (LAB1; 2 credits);
- complete the written examination which covers the fundamental knowledge in multi-scale modeling (TEN1; 3 credits);
- fulfill 2 projects by applying the knowledge learned from the "Multi-scale modeling" course to solve some practical problems in chemistry and biology (PRO1 and PRO2, together 3 credits).

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.