KTH Computational Science and Engineering Centre (KCSE)
HERO-M Centre
Department of Materials Science and Engineering, KTH

PM

4H5919 Computational Techniques in Materials Science, 9hp

Course coordinator: Joakim Odqvist (joakim@mse.kth.se)

Examiner: Prof. John Ågren (john@mse.kth.se)

Goals

After completing the course the students should be able to

- Describe different computational techniques in common use in the field of materials science and discuss their differences when it comes to physical basis and computer implementation.
- For a given problem choose a suitable numerical method, know how to use it in a simple case, interpret the results, and understand the strengths and limitations of the method. For certain methods, the student should be able to implement it in e.g. Matlab.

Contents

Overview of the field of computational materials science. Phase-field crystal modelling. Ab-initio based methods to calculate materials properties. The Calphad method and computational thermodynamics. Diffusion-controlled phase transformations and moving boundary problems. The phase-field method for simulating microstructure evolution. Molecular dynamics. Modelling of mechanical properties using FEM.

Lectures

The course consists of 9 lectures where different computational techniques in materials science will be presented. The first lecture gives an overview of the area.

Home assignments

For each lecture, except the first one, there will be a home assignment to be handed in by the student. In the home assignment your task is typically to implement a numerical method to solve a set of governing equations describing a certain phenomena of interest in

materials science. In certain cases you should use existing software and do some calculations. A total of 8 home assignments will be given. Each home assignment will be discussed at a seminar where the students are asked to present their solution.

There is no written exam but the home assignments must be handed in and approved within two months after the final lecture.

Prerequisites

All students with an interest in materials science and numerical methods are welcome to participate. However, some basic knowledge of materials science, physics and numerical methods is required.

Literature

Material handed out.

Schedule

1. Introduction to computational materials science – Prof. John Ågren, KTH

Wednesday 15/12, 14-15

2. Phase-field crystal modelling – Prof. Ken Elder, Oakland Univ., USA

Wednesday 15/12, 15-17. Seminar on the home assignment Friday 14/1, 10-12

3. Solving time dependent parabolic PDEs – Assoc. Prof. Lennart Edsberg, KTH

Friday 14/1, 13-15. Seminar on the home assignment 28/1, 10-12.

4. Simulation of diffusion and phase transformations using sharp interface models – Dr. Lars Höglund, KTH

Friday 28/1, 13-15. Seminar on the home assignment 11/2, 10-12

5. Computational thermodynamics – Assoc. Prof. Malin Selleby, KTH

Friday 11/2, 13-15. Seminar on the home assignment 24/2, 10-12

6. Introduction to electronic structure calculations using density functional theory – Assoc. Prof. Anna Delin, KTH

Friday 11/3, 13-15. Seminar on the home assignment 25/3, 10-12

7. Phase-field modelling – Dr. James Warren, NIST, USA

Friday 25/3, 13-15. Seminar on the home assignment 8/4, 10-12

8. From electronic structure to molecular dynamics - Dr. Pavel Korzhavyi

Friday 8/4, 13-15. Seminar on the home assignment 29/4, 13-15

9. Modelling of mechanical properties using FEM – Prof. Per-Lennart Larsson, KTH

Friday 29/4, 10-12. Seminar on the home assignment 13/5, 10-12