MATH-500

Error control in scientific modelling

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Cursus	Sem.	Type
Materials Science and Engineering		Obl.
Materials Science and Engineering	MA1, MA3	Opt.
Mathématicien	MA1, MA3	Opt.

Language of teaching	English
Credits	5
Session	Winter
Semester	Fall
Exam	During the semester
Workload	150h
Weeks	14
Hours	**4 weekly**
Lecture	2 weekly
Exercises	2 weekly
Number of positions	

Summary

Errors are ubiquitous in computational science as neither models nor numerical techniques are perfect. With respect to eigenvalue problems motivated from materials science (transfer problems, atomistic modelling) we discuss, implement and apply numerical techniques for estimating simulation error.

Content

- Types of simulation error
- Important eigenvalue problems in materials science
- Residual-error relationships for eigenvalue problems
- Perturbation theory
- Plane-wave basis sets and their discretisation error
- Parametrised eigenvalue problems
- Errors due to uncertain parameters: Perturbative and statistical approaches
- Non-linear eigenvalue problems (if time permits)

Learning Prerequisites

Required courses

- Analysis
- Linear algebra
- Exposure to numerical linear algebra
- Numerical methods for solving partial differential equations (such as finite-element methods, plane-wave methods)
- Exposure to implementing numerical algorithms (e.g. using Python or Julia)

This course delivers a mathematical viewpoint on materials modelling and it is explicitly intended for an interdisciplinary student audience. To keep it accessible, the key mathematical and physical concepts will both be revised as we go along. However, the learning curve will be steep and an interest to learn about the respective other discipline is required. The problem sheets and the projects require a substantial amount of work and feature both theoretical (proof-oriented) and applied (programming-based and simulation-based) components. While there is some freedom for students to select their respective focus, students are encouraged to team up across the discplines for the course work.

Teaching methods

Lectures + exercises

Expected student activities

Students are expected to attend lectures and participate actively in class and exercises. Exercises will include theoretical, programming and simulation-based assignments. Students also complete substantial group projects that contain (to varying extend) theoretical and applied components.

Assessment methods

Exercise sheets and projects