EPFL

MATH-500

Error control in scientific modelling

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Cursus	Sem.	Type
Computational science and Engineering	MA1, MA3	Opt.
Computational science and engineering minor	H	Opt.
Ing.-math	MA1, MA3	Opt.
Materials Science and Engineering	MA1, MA3,	Opt.
Mathématicien	MA1, MA3	Opt.

Language of teaching	English
Credits	5
Session	Winter
Semester	Fall
Exam	Oral
Workload	150h
Weeks	14
Hours	**4 weekly**
Courses	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 and atomistic modelling we discuss, implement and apply numerical techniques for estimating simulation error.

Content

- Important eigenvalue problems in materials science
- Motivation for studying errors in eigenvalue problems
- Types of simulation error
- Residual-error relationships for eigenvalue problems
- Perturbation theory and parametrised eigenvalue problems
- Subtleties of infinite-dimensional eigenvalue problems
- Discretisation and discretisation error
- Plane-wave basis sets
- Errors due to uncertain parameters (if time permits)
- Estimating errors in non-linear eigenvalue problems (if time permits)

Learning Prerequisites

Required courses

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

Past participants from materials science found it further useful to take this course after they followed the lectures on Statistical Mechanics or Fundamentals of solid state materials.
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 project 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.

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 project that contain (to varying extend) theoretical and applied components.

Assessment methods

Project during the semester and oral exam

Resources

Bibliography

There is no single textbook corresponding to the content of the course. Parts of the lectures have substantial overlap with the following resources, where further information can be found.

- Youssef Saad. *Numerical Methods for Large Eigenvalue Problems*, SIAM (2011).
- Nicholas J. Higham. *Accuracy and Stability of Numerical Algorithms*, SIAM (2002).
- Peter Arbenz. *Lecture notes on solving large scale eigenvalue problems*, ETHZ.
- Mathieu Lewin. *Théorie spectrale et mécanique quantique*, Springer (2022).

Ressources en bibliothèque

- [External resource] Lecture notes on solving large scale eigenvalue problems / Arbenz
- Find the references at the Library

Websites

- https://matmat.org/teaching/error-control

Moodle Link

- https://go.epfl.ch/MATH-500