PHYS-339

Advanced computational physics

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Cursus	Sem.	Type
Physics	BA6	Opt.

Language of teaching	English
Credits	3
Session	Summer
Semester	Spring
Exam	During the semester
Workload	90h
Weeks	14
Hours	**3 weekly**
Lecture	1 weekly
Project	2 weekly
Number of positions	

Summary

The course covers dense/sparse linear algebra, variational methods in quantum mechanics, and Monte Carlo techniques. Students implement algorithms for complex physical problems. Combines theory with coding exercises. Prepares for research in computational physics and related fields.

Content

Dense Linear Algebra:

- Linear systems: Upper triangular matrix inversion, QR decomposition
- Eigenvalue problems: QR algorithm
- Physical applications: Electrical Circuits, Fitting, Harmonic oscillations, Slater determinants in quantum mechanics

Sparse Linear Algebra:

- Properties and implementation of sparse matrices
- Applications to Ordinary Differential Equations (ODEs)
- Conjugate gradient method for linear systems
- Power method for eigenvalue problems
- Physical applications: Poisson Equation, Time-dependent and time-independent Schrödinger equations

Linear Variational Methods:

- Static Galerkin method: Variational ansatz, generalized eigenvalue problems
- Time-dependent Galerkin method: Linear ansatz tangent space, introduction to time-dependent variational principle
- Physical applications: Quantum Anharmonic oscillator (ground state and dynamics)

Monte Carlo Methods:

- Markov chains and detailed balance
- Metropolis-Hastings algorithm
- Parallel tempering
- Physical applications: Statistical physics of the Ising and Potts models

Learning Prerequisites

Required courses

1st and 2nd years (numerical) physics courses

Important concepts to start the course

Familiarity with Python is not compulsory at the beginning, but strongly suggested. It will be crucial during the course in order to develop the proposed exercises.

Learning Outcomes

By the end of the course, the student must be able to:

- Choose to solve a problem in physics
- Integrate appropriate numerical algorithms to solve problems
- Compare different computational methods
- Produce efficient computer codes

Teaching methods

Ex cathedra presentations, exercises and work under supervision

Assessment methods

2 written reports during the semester

Resources

Bibliography

- Press, W. H., et al. (2007). Numerical Recipes: The Art of Scientific Computing (3rd ed.). Cambridge University Press.

- Stickler, B. A., & Schachinger, E. (2022). Basic Concepts in Computational Physics (2nd ed.). Springer.

- Krauth, W. (2006). Statistical Mechanics: Algorithms and Computations. Oxford University Press.

Ressources en bibliothèque

- Numerical Recipes: The Art of Scientific Computing / Press
- Statistical Mechanics: Algorithms and Computations / Krauth
- Basic Concepts in Computational Physics / Stickler & Schachinger

Notes/Handbook

Detailed Lecture Notes will be Provided.

Moodle Link

- https://go.epfl.ch/PHYS-339