GHENT UNIVERSITY

Course Specifications

Valid in the academic year 2023-2024

Computational Physics (C001827)

Course size *(nominal values; actual values may depend on programme)*

Credits 6.0 **Study time 180 h**

Course offerings and teaching methods in academic year 2023-2024

A (semester 1)	Dutch	Gent	lecture seminar

Lecturers in academic year 2023-2024

Ryckebusch, Jan	WE05	lecturer-in-charge
Verstraelen, Toon	WE05	co-lecturer

Offered in the following programmes in 2023-2024	crdts	offering
Master of Science in Teaching in Science and Technology(main subject Physics and Astronomy)	6	A
Master of Science in Physics and Astronomy	6	A

Teaching languages

Dutch

Keywords

Computational Physics, numerical and simulation techniques, algorithms, uncertainty quantification

Position of the course

Only a restricted amount of problems in physics can be efficiently solved in an analytical fashion. A wide variety of physical problems, however, can be efficiently solved with the aid of computer simulations, numerical techniques and physics-based algorithms. Often, computational physics is considered as a third leg in physics next to theoretical and experimental physics. The course aims at introducing and describing the methodology of computational physics. This is done by means of detailed examples stemming from quantum mechanics, statistical physics, and solid-state physics. The focus of the course is NOT on computer programming, but on outlining how one can conduct physics on a computer.

Contents

A selection of the Physics's problems that are addressed in the course:
* Quantum scattering in a spherically symmetric potential
* The variational technique to solve the Schrodinger equation
* Random systems (random walks, diffusion and the arrow of time, percolation)
* Simulations in classical molecular dynamics (phases and phase transitions, diffusion, correlation functions, autocorrelation functions)
* Quantummechanical electronic structure computations of atoms and molecules
*The Monte-Carlo technique applied to spin systems and to liquids
Numerical methods which are discussed are: iterative procedure for special functions, finding the root and optimum of a function, numerical integration and differentiation, solving differential equations (Runge-Kutta methods, Verlet algorithms, Numerov technique), matrix manipulations, random number generators, Gaussian integrals, symplectic integrator, numerical quadrature, Markov chain Monte Carlo (MCMC) technique, importance sampling in high-dimensional spaces, variational optimalisation

Initial competences

Good knowledge of quantum mechanics and statistical physics.

Final competences

1 Deep knowledge of modelling and simulation techniques.
2 To be able to independently understand a physical problem and propose a solution using the computer. To be able to test physical laws with the aid of the computer ("computer experiments").
3 To introduce students to numerical techniques which are applied in solving physics's problems of current interest.

Conditions for credit contract

Access to this course unit via a credit contract is determined after successful competences assessment

Conditions for exam contract

This course unit cannot be taken via an exam contract

Teaching methods

Seminar, Lecture, Independent work

Extra information on the teaching methods

Problem sessions : in groups of a few students

Learning materials and price

All course materiaal is available free of charge at the university's electronic learning platform.
Compulsory textbook : J.M. Thijssen "Computational Physics" (Cambridge University Press, 1999, ISBN 0 521 57588 5) (Estimated Cost for Paperback is 80 EUR; E-book for 40 Euro)

References

1 J.M. Thijssen *"Computational Physics"* (Cambridge University Press, Second Edition, 2007)
2 Nicolas J. Giordano and Hisao Nakanishi *"Computational Physics: second edition"* (Prentice Hall, 2006)
3 Mark Newman *"Computational Physics"* (Createspace Independent Publishing, 2013)
4 Luca Bottcher and Hans J. Herrmann *"Computational Statistical Physics"* (Cambridge University Press, 2021)
5 Rubin H. Landau, Manuel J. Paez, and Cristian C. Bordeianu *"Computational Physics: Problem Solving with Python"* (Wiley, 2015)

Course content-related study coaching

The lecturer offers the possibility to discuss the course material with individual or small groups of students.

Assessment moments

end-of-term assessment

Examination methods in case of periodic assessment during the first examination period

Oral assessment, Assignment

Examination methods in case of periodic assessment during the second examination period

Oral assessment, Assignment

Examination methods in case of permanent assessment

Possibilities of retake in case of permanent assessment

not applicable

Extra information on the examination methods

Students are marked on the quality of a computational physics's project AND their presentation thereof. In this way, students are taught how to adequately report on scientific results.

Calculation of the examination mark

Oral examination (50%) + assignment (50%). Students who pass the assignment part (50%) of the exam but do not obtain a full credit for the course can opt to keep the mark for the assignment part during the retakes. The last obtained exam mark counts for the calculation of the final result.