GHENT UNIVERSITY

Course Specifications

Valid in the academic year 2018-2019

Computational Physics (C001827)

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

Credits	6.0	Study time	180 h
Contact hrs	52.5 h		

Course offerings and teaching methods in academic year 2018-2019

A (semester 1)	Dutch	lecture	30.0 h
		seminar: practical PC room classes	22.5 h

Lecturers in academic year 2018-2019

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

Offered in the following programmes in 2018-2019	crdts	offering
Master of Science in Physics and Astronomy	6	A
Master of Science in Engineering Physics	6	A

Teaching languages

Dutch

Keywords

Computational Physics, numerical and simulation techniques

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 and numerical techniques. 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

Physics's problems
* 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
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

Initial competences

Good knowledge of quantum mechanics and statistical physics.

Final competences

1 Acquaint the student with 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

Lecture, seminar: practical PC room classes

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.
Recommended textbook : J.M. Thijssen "Computational Physics" (Cambridge University Press, 1999, ISBN 0 521 57588 5) (Estimated Cost is 60 EUR)
Printed course material will be provided

References

1) J.M. Thijssen "Computational Physics" (Cambridge University Press, Second Edition, 2007, ISBN-13 978-0-521-)
2) Nicolas J. Giordano and Hisao Nakanishi "Computational Physics: second edition" (Prentice Hall, London, 2006, ISBN 0-13-146990-8)

Course content-related study coaching

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

Evaluation methods

end-of-term evaluation

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

Oral examination, assignment

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

Oral examination, assignment

Examination methods in case of permanent evaluation

Possibilities of retake in case of permanent evaluation

not applicable

Extra information on the examination methods

Non-periodical evaluation: 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%)