

Computational Physics (C004504)

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

Credits 6.0

Study time 180 h

Course offerings in academic year 2025-2026

A (semester 1)

English

Gent

Lecturers in academic year 2025-2026

Verstraelen, Toon

WE05

lecturer-in-charge

Caluwaerts, Steven

WE05

co-lecturer

Offered in the following programmes in 2025-2026

Master of Science in Teaching in Science and Technology(main subject Physics and Astronomy)

crdts

offering

6

A

Master of Science in Physics and Astronomy

6

A

Master of Science in Physics and Astronomy

6

A

Exchange Programme in Physics and Astronomy (Master's Level)

6

A

Teaching languages

English

Keywords

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

Position of the course

Only a limited number of physics problems have analytical solutions. Many physical problems can be solved efficiently with the help of computer simulations, numerical techniques and physics-based algorithms. Hence, computational physics is often considered a third branch in addition to theoretical and experimental physics. A kaleidoscopic overview of the main methods in computational physics is given. Within the context of this course unit, examples from quantum mechanics, statistical physics, solid state physics, and weather and climate modeling are detailed. This is not a "programming" course unit, but rather a course that demonstrates, using concrete examples from contemporary physics, how to do physics using a computer.

Contents

The physics problems covered are:

- The variational technique for numerically solving the Schrödinger equation.
- Simulations in classical molecular dynamics (thermodynamic ensembles, phases, diffusion, correlation functions, Longfin dynamics)
- Quantum mechanical electronic structure calculations of atoms and molecules
- The Monte-Carlo method applied to spin systems and fluids
- Weather and climate modeling

Thereby, the following numerical techniques are addressed: iterative procedures for special functions, determining the roots and maxima of a function, numerical integration and differentiation, solving ordinary differential equations (Runge-Kutta method, Verlet algorithms), numerical operations with matrices, generating random numbers, Gaussian integrals, symplectic integrators, Markov chain Monte Carlo (MCMC) method, importance sampling in high-dimensional spaces, variational optimization, fast Fourier transform.

Initial competences

Good knowledge of quantum mechanics and statistical physics.

Final competences

- 1 Explain, explain and justify modeling and simulation techniques from their theoretical description.
- 2 Independently understand a physical problem and prepare a computational solution.
- 3 Know and apply numerical techniques relevant to problems in Physics and Astronomy.
- 4 Physical laws and hypothesis testing using the computer (computer experiments).

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

Extra information on the teaching methods

Theory classes are given in the form of lectures.

Tutorial classes consist of supervised and independent solving of computational projects in which the theory is applied.

Study material

Type: Handbook

Name: Computational Physics
Indicative price: € 63
Optional: no
Language : English
Author : Jos Thijssen
ISBN : 978-1-13917-139-7
Number of Pages : 640
Oldest Usable Edition : 2
Online Available : No
Available in the Library : Yes

Type: Slides

Name: Computational Physics
Indicative price: Free or paid by faculty
Optional: no
Language : English
Number of Slides : 600
Available on Ufora : Yes
Online Available : Yes

Type: Software

Name: Jupyter Notebooks with computational assignments (tutorials)
Indicative price: Free or paid by faculty
Optional: no
Available on Athena : Yes
Online Available : Yes

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

Supervised solving of computational projects. Opportunity for questioning before, during and after class, and online.

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

- Theory: oral questioning with written preparation. Understanding of theory, in particular physical and computational aspects, is probed. For this part, students may use handouts from the lectures, a copy of which will be provided by the instructors. Other course materials may not be consulted during the examination.
- Assignment: oral presentation and defense. Evaluation criteria take into account the quality of presentation, taking initiative, employing technical skills and appropriate research attitude.

Calculation of the examination mark

Theory exam (50%) + assignment (50%). Students who pass the assignment do not have to retake it during the second examination period. However, you still have the right to take retake the entire second examination if you have not yet passed the entire course unit. The last grade obtained counts when calculating the final result.

Facilities for Working Students

no extra facilities