

Python for Scientists (C004212)

Due to Covid 19, the education and evaluation methods may vary from the information displayed in the schedules and course details. Any changes will be communicated on Ufora.

Course size	<i>(nominal values; actual values may depend on programme)</i>		
Credits 5.0	Study time 150 h	Contact hrs	45.0 h

Course offerings and teaching methods in academic year 2021-2022

A (semester 1)	English	Gent	lecture	22.5 h
			project	15.0 h
			seminar: practical PC room classes	7.5 h

Lecturers in academic year 2021-2022

Verstraelen, Toon	WE05	lecturer-in-charge
Leliaert, Jonathan	WE04	co-lecturer

Offered in the following programmes in 2021-2022

	crdts	offering
Bachelor of Science in Physics and Astronomy	5	A
Exchange programme Faculty of Sciences (bachelor's level)	5	A

Teaching languages

English

Keywords

Computational Physics and Astronomy, Numerical Methods.

Position of the course

This course unit belongs to the learning pathway "Computer skills" in the Bachelor program Physics and Astronomy.

Computational methods are the "bicycles of the mind": computational algorithms offer new opportunities in experimental setups or in simulations of theoretical models, all of which would be unthinkable with simple manual calculation, a calculator or a spreadsheet. Therefore, creative application of programming skills and software libraries form an important set of skills for students in the Physics and Astronomy program. These skills will prove helpful in the remainder of the study program and they are also strongly appreciated assets on the job market. This course will provide a basic theoretical understanding of numerical algorithms and their relevance to physics and astronomy. Hands-on sessions and projects during the term will complement the theory with hands-on skills to tackle various problems in the domain with computational methods. This course intends to bridge the gap between the basic course on programming (1st bachelor) and the course Computational Physics (master).

Contents

Theory:

- 1 Numerical limitations: precision (representation of floating point numbers), cpu speed (timing of algorithms) and memory (profiling).
- 2 Basic numerical building blocks in Python: lists versus arrays, mathematical array operations (element-wise and contractions), other operations (sorting, slicing, ...).
- 3 Basic visualization with 2D graphics: curves, bars, scatter plots, legends and axes, histograms, contour plots, heatmaps.
- 4 Professional programming practices: source code revisions, quality assurance

- 5 Numerical linear algebra: decompositions (QR, LU, Eigen, SVD) and solving linear problems.
 - 6 Interpolation and data modeling: multidimensional linear regression, cubic splines, chebyshev Interpolation and regularization, kriging and kernel ridge regression.
 - 7 Numerical optimization: recap of terminology (stationary points, minima, saddle points, maxima), 1D and multidimensional, convexity, gradient algorithms (SD, CG, QN), gradient-free algorithms.
 - 8 Finite difference, finite element/volume and spectral methods. Application to solving ODEs.
 - 9 Fast-fourier transform.
 - 10 (Markov-Chain) Monte Carlo sampling, importance of priors.
 - 11 Advanced numerical (efficiency) topics: vectorization, computational graphs, just-in-time compilation, ...
- Project topics will be updated on a yearly basis. Each project focuses on one or two of items 5 to 10 in the list above, addressing a physics-oriented hands-on problem, also making use of the introductory points 1, 2 and 3.

Initial competences

- 1 Basic knowledge of Python programming: built-in datatypes, flow control, functions, classes, importing modules from the standard library.
- 2 Classical mechanics, elektromagnetism, calculus, linear algebra and other basic physics and math courses will be needed in projects.

Final competences

- 1 Understand numerical limitations: precision and available resources (cpu time, memory, ...).
- 2 Understand working principles, strengths and limitations of computer algorithms used in computational physics and astronomy. (See course contents for more details.)
- 3 Tackle basic computational problems by programming in Python, mainly using NumPy and SciPy.
- 4 Know available Scientific programming libraries and find required functions or classes in their documentation.
- 5 Process input data coming from various sources (CSV, TXT, HDF5, NPZ) and output raw results in the same formats.
- 6 Create insightful visualizations of input data or computational results (2D plotting).
- 7 Basic understanding of Unix and HPC. Installation of a Python development environment on any operating system of 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, project, seminar: practical PC room classes

Learning materials and price

Syllabus in the form of Python notebooks, available on Ufora.

References

- Strongly recommended: Scientific Computing, An Introductory Survey, Revised Second Edition – Michael T. Heath
- Other useful books: Numerical Recipes in Python

Course content-related study coaching

Website (Ufora) with additional material and references available. Ample opportunity for asking questions, both personally and by electronic mail.

Evaluation methods

end-of-term evaluation and continuous assessment

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

Oral examination

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

Oral examination

Examination methods in case of permanent evaluation

Assignment

Possibilities of retake in case of permanent evaluation

examination during the second examination period is not possible

Extra information on the examination methods

- Closed-book theory exam (end-of-term evaluation) will evaluate mainly points 1 and 2 of the final competences. Insight into these topics is required, whereas reproduction of theoretical is less critical.
- Permanent evaluation on active participation in the computational projects during term, showing creative input and constructive peer assessment. Mistakes and errors due to experimentation are allowed (encouraged even) without any repercussions in the final score.

Calculation of the examination mark

- 50% theory (end-of-term evaluation)
- 50% active project participation (permanent evaluation)
- Students who eschew period-aligned and/or non-period-aligned evaluation may be failed by the examiner.