UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

COURSE SYLLABUS

Elements of Programming Languages for Materials Science

2526-3-ESM01Q020

Aims

This course aims to provide students with a solid and well-structured foundation in Python programming, with a specific focus on applications in Materials Science. In addition to acquiring proficiency in syntax and programming logic (Dublin Descriptor 1: Knowledge and understanding), students will learn how to design and implement customized tools for data analysis, numerical modeling, and simulation of physico-chemical systems (Dublin Descriptor 2: Applying knowledge and understanding).

An additional goal is to introduce the use of Artificial Intelligence tools to accelerate and optimize code development, improving the efficiency and adaptability of computational solutions. This encourages students to critically engage with emerging technologies and supports the development of independent learning strategies (Dublin Descriptor 5: Learning skills, and 3: Making judgments).

Through real-world-inspired examples and exercises, the course fosters a practical and creative programming mindset, enabling students to tackle complex scientific problems autonomously and to communicate effectively, including in the presentation and documentation of code and results (Dublin Descriptor 4: Communication skills).

Contents

The course introduces the principles of programming, both imperative and object-oriented, starting from the concept of algorithms and computational cost. Core concepts such as variables, data types, control structures, functions, and input/output operations will be presented.
Building on these foundations, students will develop simple programs with practical applications in Materials Science, including simulations, data handling and processing, and the automation of repetitive tasks.
In the final part of the course, AI-assisted programming techniques will also be discussed.
The programming language used throughout the course is Python.

Detailed program

1. Programming fundamentals: Introduction to core concepts such as variables, data types, input/output operations, control structures, and functions.
2. Data handling: Manipulation of data using lists, dictionaries, and arrays. Introduction to libraries for numerical computing and data analysis.
3. Data visualization: Creating plots and visual representations to support the analysis of experimental results and scientific simulations.
4. Introduction to modeling: Basic principles of scientific simulation, including Monte Carlo methods and the implementation of simple algorithms.
5. Automation and scripting: Writing scripts to automate repetitive tasks, such as processing large datasets or interfacing with scientific instruments.
6. AI-assisted programming: Developing code with the support of artificial intelligence tools to accelerate and optimize the coding process.

Prerequisites

A basic knowledge of mathematics is required. While a good understanding of previous Materials Science courses can help in better appreciating the purpose of the programs developed during the course, it is not essential. No prior programming experience is required.

Teaching form

Instructional teaching: Lectures (3 CFU, 24h).
Interactive teaching: Laboratory activity (3 CFU, 36h).

Lectures are given in Italian.

Textbook and teaching resource

Two freely available books for learning to program in Python are:

1. "Think Python" by Allen B. Downey (http://greenteapress.com/wp/think-python-2e)

2. "Automate the Boring Stuff with Python" by Al Sweigart (https://automatetheboringstuff.com — available to read online for free or to purchase on Amazon)

Additional materials will be provided during the course.

Semester

Second semester.

Assessment method

The final assessment consists of a written test and an oral exam.

The written test involves writing a few short Python programs, aimed at evaluating the student's grasp of basic programming concepts.

The oral exam includes a discussion of a project previously agreed upon with the instructor, as well as questions on the course content.

No midterm exams are scheduled.

Office hours

Available daily by appointment.

Sustainable Development Goals

QUALITY EDUCATION