



## COURSE CARD

### 1. Basic information

|                                                                                                                                        |                                                                       |                                     |
|----------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------|-------------------------------------|
| Course name in English:                                                                                                                | Introduction to Python for Scientific Calculations                    |                                     |
| Course name in Polish:                                                                                                                 | Wprowadzenie do Pythona do obliczeń naukowych                         |                                     |
| Number of hours:                                                                                                                       | 15                                                                    |                                     |
| Type of course:                                                                                                                        | Elective course                                                       |                                     |
| Form of course:                                                                                                                        | laboratory                                                            |                                     |
| Code of course:                                                                                                                        |                                                                       |                                     |
| Course leader:                                                                                                                         | dr Justyna Rogacka                                                    |                                     |
| Faculty of the course leader:                                                                                                          | W3 Faculty of Chemistry                                               |                                     |
| Email address of the course leader:                                                                                                    | justyna.rogacka@pwr.edu.pl                                            |                                     |
| Scientific discipline(s) assigned to the course (doctoral students representing the marked disciplines can participate in the course): | Architecture and urban planning                                       | <input type="checkbox"/>            |
|                                                                                                                                        | Automation, electronic, electrical engineering and space technologies | <input checked="" type="checkbox"/> |
|                                                                                                                                        | Information and communication technology                              | <input checked="" type="checkbox"/> |
|                                                                                                                                        | Biomedical engineering                                                | <input checked="" type="checkbox"/> |
|                                                                                                                                        | Chemical engineering                                                  | <input checked="" type="checkbox"/> |
|                                                                                                                                        | Civil engineering, geodesy and transport                              | <input checked="" type="checkbox"/> |
|                                                                                                                                        | Materials engineering                                                 | <input checked="" type="checkbox"/> |
|                                                                                                                                        | Mechanical engineering                                                | <input checked="" type="checkbox"/> |
|                                                                                                                                        | Environmental engineering, mining, and energy                         | <input checked="" type="checkbox"/> |
|                                                                                                                                        | Mathematics                                                           | <input type="checkbox"/>            |
|                                                                                                                                        | Chemical sciences                                                     | <input checked="" type="checkbox"/> |
|                                                                                                                                        | Physical sciences                                                     | <input checked="" type="checkbox"/> |
|                                                                                                                                        | Management and quality studies                                        | <input checked="" type="checkbox"/> |

### 2. Objectives

The aim of this course is to equip PhD researchers with the skills to use Python effectively for scientific calculations and data-driven research. By the end of the course, students will be able to use core Python syntax and key scientific libraries to carry out numerical analysis, visualise data, and implement basic numerical methods such as optimisation, regression, and solving differential equations. They will learn to structure reproducible code using functions, scripts, and apply Python to discipline-specific problems in chemistry, physics, engineering, economics, and statistics. Students will also gain experience automating routine research tasks and will complete a small independent computational project relevant to their field.

### 3. Content

*Detailed information about the course content, including topics and form of classes.*



| No. | Topic                                             | Number of hours | Form of classes |
|-----|---------------------------------------------------|-----------------|-----------------|
| 1   | Python Foundations                                | 2               | laboratory      |
| 2   | Scientific Programming and Reproducible Workflows | 2               | laboratory      |
| 3   | Statistics and Data Analysis                      | 2               | laboratory      |
| 4   | Chemistry Applications                            | 2               | laboratory      |
| 5   | Physics Applications                              | 2               | laboratory      |
| 6   | Engineering Applications                          | 2               | laboratory      |
| 7   | Economics and Finance Applications                | 2               | laboratory      |
| 8   | Project Presentations                             | 1               | laboratory      |
| 9   |                                                   |                 | Select form     |
| 10  |                                                   |                 | Select form     |
| 11  |                                                   |                 | Select form     |
| 12  |                                                   |                 | Select form     |
| 13  |                                                   |                 | Select form     |
| 14  |                                                   |                 | Select form     |
| 15  |                                                   |                 | Select form     |

#### 4. Prerequisites

*List of prerequisites relating to knowledge, skills and other competences for course participants.*

Participants are expected to have a basic understanding of undergraduate-level mathematics (algebra, calculus, and simple differential equations) and familiarity with scientific problem-solving in their own discipline. No prior programming experience is required, though previous exposure to any programming language will be helpful. Students should be comfortable working with data, interpreting graphs, and engaging with computational approaches relevant to their research area.

#### 5. Learning outcomes

*List of learning outcomes at level 8 of the Polish Qualifications Framework assigned to the course (mark the learning outcomes in the last column).*

| Symbol | Learning outcome                                                                                                                                                         |                                     |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------|
|        | <b>KNOWLEDGE.</b> Doctoral student knows and understands:                                                                                                                |                                     |
| SzD_W3 | the main trends in the development of the scientific or artistic disciplines covered in the curricula;                                                                   | <input checked="" type="checkbox"/> |
| SzD_W4 | research methodology;                                                                                                                                                    | <input checked="" type="checkbox"/> |
| SzD_W5 | the rules for the dissemination of scientific results, including in open access mode;                                                                                    | <input type="checkbox"/>            |
| SzD_W6 | the fundamental dilemmas of modern civilization;                                                                                                                         | <input type="checkbox"/>            |
| SzD_W7 | the legal and ethical conditions of scientific activity;                                                                                                                 | <input type="checkbox"/>            |
| SzD_W8 | the economic and other relevant conditions of scientific activity;                                                                                                       | <input type="checkbox"/>            |
| SzD_W9 | basic principles of knowledge transfer to the economic and social spheres and commercialisation of results of scientific activity and know-how related to these results. | <input type="checkbox"/>            |



|        | <i>SKILLS. Doctoral student is able to:</i>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                                     |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------|
| SzD_U2 | use knowledge from different fields of science or art to creatively identify, formulate and innovatively solve complex problems or perform research tasks, in particular:<br>- define the purpose and subject of scientific research, formulate a research hypothesis,<br>- develop research methods, techniques and tools, and use them creatively,<br>- draw conclusions on the basis of scientific research;<br>critically analyse and evaluate the results of scientific research, expertise and other creative work and their contribution to knowledge development;<br>transfer the results of scientific activities to the economic and social spheres; | <input checked="" type="checkbox"/> |
| SzD_U3 | communicate on specialised topics to the extent that they enable an active participation in the international scientific community;                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | <input type="checkbox"/>            |
| SzD_U4 | disseminate research results, including in popular forms;                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | <input type="checkbox"/>            |
| SzD_U5 | initiate debates and participate in a scientific discourse;                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | <input type="checkbox"/>            |
| SzD_U6 | be able to speak a foreign language at B2 level of the Common European Framework of Reference for Languages to a level that enables them to participate in the international scientific and professional environment;                                                                                                                                                                                                                                                                                                                                                                                                                                          | <input type="checkbox"/>            |
| SzD_U7 | plan and implement an individual or collective research or creative activity, including in an international environment;                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | <input type="checkbox"/>            |
| SzD_U8 | independently plan and act for one's own development and inspire and organize the development of others;                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | <input type="checkbox"/>            |
| SzD_U9 | plan classes or groups of classes and implement them using modern methods and tools.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | <input checked="" type="checkbox"/> |
|        | <i>SOCIAL COMPETENCES. Doctoral student is ready to:</i>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                     |
| SzD_K3 | fulfilling the social obligations of researchers and creators, initiate public interest activities, thinking and acting in an entrepreneurial way;                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | <input type="checkbox"/>            |
| SzD_K4 | maintaining and developing the ethos of research and creative environments, including:<br>- carrying out scientific activities in an independent manner,<br>- respecting the principle of public ownership of research results, taking into account the principles of intellectual property protection.                                                                                                                                                                                                                                                                                                                                                        | <input checked="" type="checkbox"/> |

## 6. Evaluation

*Short description of the method(s) used to evaluate the learning outcomes assigned to the course, e.g., exam, test, report, presentation, etc.*

Project preparation and presentation

## 7. Teaching methods

*Short description of the teaching methods used during the course, e.g., multimedia presentation, discussion, literature studies, developing written documents, own work, etc.*

Computer laboratory based on live coding demonstrations

## 8. Literature



*List of primary and secondary literature used to prepare the course and including additional knowledge for participants, e.g., books, textbooks, research papers, standards, web pages, etc.*

1. Johansson, Robert. *Numerical Python: Scientific Computing and Data Science Applications with NumPy, SciPy and Matplotlib*. Apress / Springer, 2024.
2. VanderPlas, Jake. *Python Data Science Handbook: Essential Tools for Working with Data*. O'Reilly Media, 2016 (2nd edition: 2023).
3. VanderPlas, Jake. *Python Data Science Handbook — online version* (Jupyter notebooks + web) [online resource]. Available at: <https://jakevdp.github.io/PythonDataScienceHandbook/>

## **9. Other remarks**

*Additional remarks, comments, (e.g., language of the course)*

English language