CK1310 Python Programming for Chemical Sciences 3.0 credits

Programmering i Python inom kemivetenskap

This is a translation of the Swedish, legally binding, course syllabus.

If the course is discontinued, students may request to be examined during the following two academic years

Establishment
Course syllabus for CK1310 valid from Autumn 2023

Grading scale
A, B, C, D, E, FX, F

Education cycle
First cycle

Main field of study
Technology

Specific prerequisites
SF1625 Calculus in one variable
Language of instruction
The language of instruction is specified in the course offering information in the course catalogue.

Intended learning outcomes
After course completion, the student shall demonstrate skills and ability by

• Implementing a basic mathematical model with theoretical chemistry in a well structured program written in Python
• Showing ability to present goals, implementation, and results of a programming project in written form

Course contents
The course provides basic knowledge about mathematical modeling, numerical methods and their role and function for chemistry applications, and structured programming for implementation of mathematical models. The course projects target areas closely related to chemistry.

The course contains:

• A discussion about the role of modeling in chemistry
• Design of a project in chemistry with focus on mathematical modeling
• Implementation in Python of a numerical model
• Literature study and handling of references
• Self reflection based on group dynamics and processes
• Report writing

Examination
• PRO1 - Project, 3.0 credits, grading scale: A, B, C, D, E, FX, F
Based on recommendation from KTH’s coordinator for disabilities, the examiner will decide how to adapt an examination for students with documented disability.

The examiner may apply another examination format when re-examining individual students.

Ethical approach
• All members of a group are responsible for the group’s work.
• In any assessment, every student shall honestly disclose any help received and sources used.
• In an oral assessment, every student shall be able to present and answer questions about the entire assignment and solution.