Scientific Programming Methods for Chemists

Module	Credits	Workload	Term	Frequency	Duration
13 EC	5 CP	150 h	2. Sem.	SuSe	1 Semester

Courses	Contact hours	Self-Study	Group size
a) Lecture b) Exercises	a) 2 SWS b) 1 SWS	a) 30 h b) 75 h	10-20 Students

Prerequisites

None

Learning outcomes

After successful completion of the module students will:

- have basic knowledge programming concepts of modern programming languages
- know how to structure code and how to test and validate source code
- be able to turn scientific modelling problems into programmable algorithms
- have some experience on how to use code libraries to solve standard mathematical problems and to visualize scientific data

Content

The lecture uses Python as an example of a modern object-oriented programming language to introduce students to:

- elementary data types (integers, floats, strings, etc.) and their representation in computers
- control structures (loops, conditions, functions, etc.)
- basics of object orientation (classes, inheritance, etc.)
- complex data types (lists, tuples, dictionaries, etc.)
- reading and writing data from/to files
- math libraries (numpy, scipy, blas, lapack)
- visualization of data with matplotlib
- solving differential equations numerically on grids
- solving algebraic problems (linear equations, SVD, eigenvalue problems)

Teaching methods

Lecture, Hands-on coding projects for self-studying on own laptops with online support by teaching assistants via a chat work space, Q&A and discussion sessions, Moodle course with online material.

Mode of assessment

submission and grading of the solution sheets for the hands-on problems and a final written or oral end-of-semester exam

Requirements for the award of credit points

successful written or oral end-of-semester exam

Module applicability

M.Sc. iMOS; M.Sc. Chemistry

Weight of the mark for the final score

by CP

Module coordinator and lecturer(s)

R. Schmid, C. Haettig