CD224 Jan 2:1
Computers in Chemistry

Instructor
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Department: IPC
Course Time: Mon and Wed: 11 am - 12 noon, Fri: 2 - 5 pm
Lecture venue: Mon and Wed: MRC Classroom, Fri: TBD

Detailed Course Page:

Announcements

Brief description of the course
The course is meant as a first programming course for students in the Int PhD programme of the Chemical Sciences division. They are introduced to the utility of coding in Python, and require no prior experience at the start of the course. Over the duration of the semester, they will get a first glimpse how to use small and efficient codes to their speed-up/benefit in their research tasks.

Prerequisites
none

Syllabus
Basic programming in Python using simple examples. Numerical methods: interpolation, numerical integration and differentiation, Gaussian quadrature, numerical methods in linear algebra, eigensolutions, special cases like Hueckel theory, linear and non-linear data fitting, solutions of ODEs, Fourier transforms

Course outcomes
The key objective of this course is to impress upon all the course students, especially experimental and theoretical chemists alike, that being able to code, even a little bit, is very useful. Although the numerical
techniques discussed are largely available in standard data processing and plotting packages like Origin or Matlab or Mathematica, it is important to know at a basic level what these packages actually do. This would help them understand what to make of the output data from the packages. Knowing to code would help them extract and process or organize data from instruments or other code efficiently, thereby becoming a useful tool in their everyday research.

**Grading policy**

50% for in-semester tests and assignments, 50% for final exam (written + practical)

**Assignments**

**Resources**

The course participants may use any useful website