

COMPUTATIONAL METHODS IN EARTH SCIENCES

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1. COURSE DESCRIPTION

The objective of this course is to introduce students to a range of ways in which computers can help them analyze and process data, translate ideas and conceptual models into computer simulations, visualize their findings, and work alone or in teams to address research questions. Students will be introduced to the Python programming language, which is easy to learn and used broadly across the geosciences. They will work with real data sets and write models to understand systems that are of relevance to their research.

2. REQUIRED MATERIALS

- Bring a laptop computer to class; please email the instructor if this is a problem
- Textbook, *Think Python: How to Think Like a Computer Scientist*: PDF and HTML available at <http://www.greenteapress.com/thinkpython/>

3. LEARNING GOALS

This course will be broken into four modules:

- (1) An introduction to the Python programming language
 - Commands in Python
 - Imperative and object-oriented programming
 - Software architecture and (re)usability
- (2) Working with data sets
 - Text files, binary data files, spreadsheets, and specialized formats (e.g., NetCDF)
 - Plotting data
 - Basic data analysis
 - Optional: Introduction to GIS applications with Python
- (3) Working with models
 - Introduction to types of models
 - Differential equations review: simple analytical solutions, Taylor series approximations, and numerical solutions
 - Matrix algebra to solve systems of differential equations: applying the finite difference method
- (4) Projects
 - Build software that will assist you in a topic of your choosing (ideally related to your research)

- Learn how to use version-control software and appropriate licensing for collaborative work
- Integration of data and models is encouraged
- Present results at the end of the semester

4. EVALUATION

Students taking the course for a grade will be evaluated on the basis of their contribution to the final project. This will include:

- Participation and course-related work through the semester (35%)
- Final project code (50%)
- Final project presentation (15%)

5. SCHEDULE

Important Note: *Due to the instructor's travel schedule, we are having only six class meetings. These will be very dense classes, and you are expected to need to take approximately the same amount of time as the class on your own to properly learn. The course notes are long and full of examples (code provided), links to on-line resources, and information on both the theory and practice of programming; these along with your textbook should be good resources for additional study. Please do not hesitate to send an email if anything in the course notes is unclear or does not work as expected; this is the first time that the class has been taught, so it is quite possible that something will need to be fixed!*

06 May, 14:00–17:00: Haus 27, Raum 2.36

Programming: philosophy, problem-solving, and basic vocabulary

Reading: Chapters 1–2

- **Before class:** Install Python Python 2.7.X on your computer. Please email the instructor if you have problems.
 - Windows and Mac: Python(x,y) is the most open-source distribution, but Anaconda is the easiest to download and use. See <http://docs.continuum.io/anaconda/install.html>
 - Linux: “apt-get install python-numpy python-scipy python-matplotlib ...” or equivalent from your package manager
- **Before class:** Also install a nice programming editor like TextWrangler (Mac), Notepad++ (Windows), or gedit (every platform)
- Editing and running Python: text editors, Spyder, iPython
- Programming syntax
- Variables and types
- Loops and statements
- Introduce version control software (goal: download course materials with git)
- Exercise: Randomly-walking particle (or something else fairly simple that applies these skills)

08 May, 08:15–12:00: Haus 25, Raum D2.01

Classes, functions, modules, plotting

- **Before class:** Version control software installed and working
- Introduction to namespaces
- Python modules (built-in)
- Functions
- Classes and object-oriented programming
- Using a pre-built module: Matplotlib for plotting

22 May, 09:15–12:00: Haus 25, Raum D2.01

Working with data

- **Before class:** Bring a set of data you want to analyze; email the instructor to ensure that your data format will be covered
- Text files
- Spreadsheets
- Binary files
- NetCDF and HDF files
- Geospatial data (if we get this far)
- Plotting data

10 June, 13:15–16:00: Haus 27, Raum 2.36

Math review; introduction to modeling; probability theory

- (1) Andy Wickert's lecture
 - Derivatives and differential operators
 - Integrals and numerical methods for integration
 - Vectors, matrices, and arrays
 - Dot products, cross products, matrix multiplication
 - Vector notation and Einstein (summation) notation
- (2) **Guest lecture:** Prof. Dr. Crystal Ng
 - Probability in the geosciences
 - Integrating data sets and models
 - Modeling hillslope evolution

12 June, 09:15–12:00: Haus 25, Raum D2.01

Modeling and finite difference methods

- Discretization with a geometric argument (out minus in)
- Discretization with Taylor Series
- Discussion of orders of numerical precision
- Forward difference (central difference) discretization of differential equations: thermal diffusion example
- Implicit solutions: implicit-in-space solution for the diffusion equation (Crank–Nicolson solutions are implicit in time as well, but I do not think we will have time to cover these)
 - (1) Building matrix solutions
 - (2) Solving a n -diagonal system of equations

19 June, 09:15–12:00: Haus 25, Raum D2.01

Final projects – start of work

This is really your day to discuss your final projects with the instructor and to make plans for how to move forward with them. These final projects are **Required for all students who are taking the courses for credit**, and should ideally include some component of your research (this is for your sake – so it is useful to you!)

*****INSTRUCTOR IN THE FIELD IN ARGENTINA 23 JUNE – 30 JULY; WILL DO HIS BEST TO ANSWER EMAILS RELATED TO FINAL PROJECTS. SO GET STARTED REALLY EARLY!*****

Please submit your final projects via GitHub and/or email. (Required only for those seeking credit; others of course are welcome to receive feedback)

First week of August: those of you who need a Prüfungsausschuss must meet with the instructor to discuss your final projects and to obtain a signed Prüfungsausschuss. These will be turned in to Apl. Prof. Dr. Martin Trauth (see <http://www.geo.uni-potsdam.de/pruefungsausschuss-1323.html> for more information). Please email Andrew Wickert (andrew.wickert@uni-potsdam.de) about this at your earliest convenience. The instructor is moving to the USA after the first week of August, so promptness is in your own best interests!