

Syllabus for PHYS 440/640: Computational Physics

TU 11:20-12:50 pm, TH 11:20-12:20 Rm 226

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1 Overview

This course is about using computers to do physics, and also to solve computational problems in other fields from a physics perspective. Note that this is NOT a computer science course. The 4 main categories of activities in this course are:

1. Getting started with Python: Arrays, scripts, random numbers, array index operations, flow control, code documentation, analyzing existing code, numerical algorithms, numerical errors, plotting.
2. Doing physics with computers; solving problems or investigating behavior of systems that have no exact analytical representation; visualization/animation for exploring data or physical concepts
3. Modeling: creating a mathematical model for a scientific problem. Defining the physics, translating to math, developing a computational algorithm, exploring parameter space, writing up results
4. Data analysis: plotting, statistical analysis, comparing to models, testing hypotheses
5. Using \LaTeX for project reports: all writeups must be in Latex. Templates and typeset pdfs will be uploaded to Bb. Contributed templates from students are encouraged.

The class format will include a lecture on the physics topic or numerical algorithm, individual/group work and student presentations. I will assume that all students have laptops and that Python is installed prior to the first class.

2 Computer languages/OS

I will assume basic familiarity with Unix; I use MAC OSX which has Unix under the hood. I have little expertise or interest in Windows, and I use IDL. My preliminary survey indicated that the majority of you have some experience with computation. The preferred language for this class is Python since it's open source, lots of resources are available, and technical computing seems to be moving in that direction. The majority of you are familiar with Python, according to my survey. For those who have never worked with it (that includes me), there are many tutorials available. I'd like to use Python 2 instead of Python 3 in case the code/packages we want to use aren't available in Python 3. We'll use the Anaconda distribution, which can be downloaded at <https://anaconda.com>.

Jupyter Notebook is a development environment that's good for beginners. It comes with the Anaconda distribution.

A few tutorials on youtube: *Python Tutorial for Absolute Beginners* <https://www.youtube.com/watch?v=Z1Yd7upQsXY> (This is a series).

Quick Introduction to Jupyter Notebook at <https://www.youtube.com/watch?v=jZ952vChhuI>.

Also <https://www.python-course.eu/course.php>

Documentation/resources: <https://www.python-course.eu/course.php>

No official textbook is required for this class, but I recommend the inexpensive paperback: *Python Programming and Visualization for Scientists*, A. De Caria, Sundog Publishing. The first 3 chapters are a free sample posted in course materials on Bb. *A hands-on introduction to using Python in the Atmospheric and Oceanic Sciences*, Johnny Lin. See Bb for free copy, payment optional, but send a few bucks if you can.

3 General computational physics topics covered will include:

- Random numbers and stochastic processes
- Numerical integration of differential equations; eigenvalue problems
- Chaos and "sensitivity to initial conditions", non-linear systems, dynamical phase space
- Monte Carlo Simulation
- Biologically and physically-inspired algorithms: genetic algorithms, wavelets and feature detection, stochastic annealing
- Data analysis: statistics, pdfs, conditional statistics, temporal/spatial scale analysis, FFT, structure functions
- Optimization problems

We'll apply these numerical tools to a variety of problems including some of the following: the nonlinear oscillator, random walks, Brownian motion, binary alloys, 2-D Ising model phase transition, percolation, diffusion-limited aggregation, reaction-diffusion systems, predator-prey models, simplified protein folding, photon scattering/the Sinai billiard problem, gas-liquid phase transition for Van der Waals gas, traffic, hydrogen atom wavefunctions, ODEs/PDEs with forcing. We may not have time to look at all of these; I encourage you to explore these or other topics of your own choosing in individual projects and HW. Additional atmospheric physics applications will be assigned for those taking 640. Data analysis assignments will emphasize tools such as correlation, conditional pdfs, fitting, a variety of techniques for torturing the data until it confesses.

4 BlackBoard

Phys 640 has a Bb site and you are encouraged to check it a couple of times a day for announcements. The discussion section will have forums on student-contributed Python tricks/code, plotting and any other topics that will need a separate forum. Each HW assignment will also have its own forum where ideas can be exchanged and questions posted. Submissions of useful scripts or \LaTeX templates that others might find useful are encouraged. Send them to me and I'll put them in course documents in the "submitted" folder. Include your initials as part of the name of the script/template.

5 Homework/projects

The homework assignments will be based on finishing work started in class. The report for each problem should include 1) an introduction (what is the purpose of the exercise), 2) code - with comments! Each portion of the code should be preceded with a statement saying what it does. Highlight those comments so they stand out); 3) results - plots, tables that display the results of the computation; 4) Discussion: discuss and explain results, e.g. the impact of changing the parameters; discuss the physics where applicable. Your written reports must be entirely your own work.

6 Grading

There will be no exams in this course. Your grade will be based on 2 class presentations (10%), 12 HW projects/assignments (60%), a longer mid-term project (10%) and an extensive final project (20%). The midterm project is due the first class after spring break. The proposal for the final project is due in mid-April, the final project is due during the last week of classes. Specific dates TBD.

7 Writing reports

All reports should be written in \LaTeX ; the mid-term and final projects must be written in a style suitable for publication. Project reports should contain an Intro/overview and motivation if relevant, code, results/plots, discussion/insights, summary and conclusions, references if applicable. The code should be placed in an appendix unless there is an important aspect of it that should be highlighted in the body of the report. There is likely a wide variation in computational expertise among you. I encourage collaboration; group discussion on strategies for code development, formulating models and other work will be part of the class meeting, but again, reports must be your own work.

7.1 Using \LaTeX for project reports

All reports on projects in this course will be typeset using \LaTeX . It's a good idea to learn how to use it; most journals will accept \LaTeX documents, and offer "style files" that automatically format the document in the style of a given journal. You should also consider using it for your thesis. There are LOTS of resources available online for \LaTeX users; good sources for \LaTeX are the Comprehensive TeX Archive Network (ctan.org) and the worldwide TeX Users Group (tug.org).

The \LaTeX distribution for both MAC and Windows can be downloaded (free) at ctan.org. For Windows, you can download the package proTeX. It includes MikTeX as the engine, and TeXstudio as the text editor.

Some other links are:

<http://miktex.org/>
<http://www.howtotex.com/howto/installing-latex-on-windows/>

The engine for MAC is TexShop. This is part of the MacTeX package and it can also be downloaded at ctan.org or tug.org (<http://tug.org/mactex/>).

<http://www.macupdate.com/app/mac/12104/texshop>

Useful Latex tutorial stuff:

<http://www.andy-roberts.net/misc/latex/index.html>
<http://ctan.tug.org/tex-archive/info/lshort/english/lshort.pdf>
<http://www.howtotex.com/packages/beautiful-matlab-figures-in-latex/>

Some of the above documents are posted on Bb: see *Course Documents*. Read "A short example of how to use \LaTeX for scientific reports". The latex archive includes everything you need to know to get started. The material there was downloaded from

<http://www.damtp.cam.ac.uk/user/eglen/texintro>.

and includes a report "template" that you can change as you see fit. I'll be adding more to the Latex folder on Bb. The final project will be written using AGU or Physical Review style files and will be written as a formal journal article.