Syllabus for PHYS 440/640: Computational Physics
12:30-3:00 pm Fridays, 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. The 4 main categories of activities in this course are:

1. Getting started with Matlab: Arrays, scripts, random numbers, array index operations, flow control, code documentation, analyzing existing code, numerical algorithms, numerical errors, convergence, plotting. Useful tricks (e.g.arrow keys).
2. Doing physics with Matlab; 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 be comprised of a short lecture, followed by individual and group work. I will assume that all students have laptops and that Matlab is installed prior to the first class. See Paul Ciotta for help on this.

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. My preliminary survey indicated that most of you have some experience with Matlab, so we'll begin with that. Matlab is widely used in both academia and industry, and in many areas of science and engineering. If time permits, I'd like to include brief modules on Mathematica and/or Python towards the end of the semester. Let's see how this goes. For those who already know these languages and would like to use them in some projects instead of Matlab, talk to me first.

2.1 Matlab for newbies

For those who have never used it, please look at the introductory materials and work through the exercises before the first day of class. Introductory tutorials can be found on Bb in the "Matlab Intro" folder in *Course Documents*. The first lecture will begin with a brief overview by a guest lecturer who uses Matlab extensively in NASA-related work.

2.2 Matlab resources

An important component of this class is using search engines such as Google/Google Scholar or the library to find any information that is relevant for the assignment or project. Lots of Matlab scripts can be found online. You must include the link and date accessed or a reference from the literature in your report. Some good resources:

MATLAB: Numerical Computing with MATLAB, by Cleve Moler. The Introduction is in *Course documents*. The book and Matlab scripts can be downloaded for free at

http://www.mathworks.com/moler/chapters.html

matlab scripts can be found at

http://www.mathworks.com/matlabcentral/fileexchange/

also take a look at
http://www.mathworks.com/matlabcentral/about/trendy/
and
http://www.mathworks.com/matlabcentral/fileexchange/23972-chebfun/content/chebfun/

No official textbook is required for this class, but there are some out there that look pretty good, e.g.
http://www.amazon.com/Matlab-Second-Practical-Introduction-Programming/dp/0123850819/ref=sr_1_1?s=books&ie=UTF8&qid=1359085168&sr=1-1&keywords=matlab
I advise against getting the Kindle versions since the graphics are poor.

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, quantum dots, optical bistability/noise-induced transitions, 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. 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 encourage to check it a couple of times a day for announcements. The discussion section will have forums on Matlab 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 Class time:

- Lecture: Brief intro to the content and learning goals for the day.
- Active learning: Setting up code structure for tackling the problems for the day. In-class coding following examples; generating preliminary results. Preliminary data analysis. The *diary on* command will open a file that will record all typed classwork, and *diary off* will write to the file and close it. This will record everything you type in class; you can add comments, and edit the file later. This file will be part of your class notes.
- Group Work: Where applicable. Some modeling problems will require you to work in groups to generate ideas.

The homework assignments will be based on finishing the 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 on March 29. The proposal for the final project is due on April 19, the final project is due on May 17.

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. Fernando Calderon has experience with the Texmaker package, he's kindly offered to help the Windows people install it.

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/`). The latest TexShop upgrade requires OS 10.7:

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

Useful 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.