Physics 3274—Computational Methods Fall Term 2016
105 Allen Hall Tuesday & Thursday 2:30-3:45
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Office hours Wed. 1:00-5:00 PM

Physics 3274 is a graduate course on computational physics. It aims to develop or reinforce programming skills, numerical analysis skills, familiarity with some important problems in computational physics and their methods of solution. Additionally, I hope it will build the student's self- confidence when confronted with computational challenges likely to arise during his/her career.

The following is a tentative schedule for the course. The qualification in the second column describes whether the lecture is mostly devoted to computing [C] , to numerical analysis [N], or to three ingredients physics [P]. As you can see the course is actually a mixture of these

1 Sep	C	Building programs in a Unix environment
3	C	Assembling larger programs. The SVN system
8	C,	Encapsulation. Built-in datatypes and classes
10	C,P	A tour of some useful class libraries
15	P	Solutions to selected undergraduate problems.
17	N	Root finding. Interpolation.
22	N	Integration with classical quadrature formulae
24	N	Gaussian Integration
29	C	How to write a class I
1 Oct	C	How to write a class II
6	N	Uniform and nonuniform variate generation.
8	N	Monte Carlo Integration & Markov Chain Monte Carlo
13	P	Percolation Theory I
15	P	Percolation Theory II
22	C	Graphics for Physicists
27	N,P	Ordinary differential equations:
29	P	Solutions to problems in classical mechanics
3 Nov	C	Polymorphism and object-oriented programming
5	P	Classical Chaos I
10	P	Classical Chaos II
12	P	Classical Spin Systems & the Ising model.
17	P	Schroedinger equation. Shooting methods and variational methods
19	P	Schroedinger equation. Matrix methods.
24	P	Hartree-Fock equations and solutions.
1 Dec	P	Rotations in quantum mechanics
3	C	Templates and the standard template library

8	P	Statistical analysis and data modeling. Basic notions. χ^2 and binned likelihood fits.
10	P	Unbinned maximum likelihood fits. Bayesian inference with Markov Chain Monte Carlo

The book:

• *Numerical Recipes, the Art of Scientific Computing, 3rd Edition*, William H. Press, Saul A. Teukolsky, William T. Vetterling, and Brian P Flannery, 2007 (Cambridge University Press).

is not employed a textbook, but rather as a critical resource which you can access while trying to solve homework problems. It will often handy not only in this course but (I believe) often throughout your career. The main reading material in the course is my lecture notes and documentation which will be circulated chapter-by-chapter as we work through the syllabus. These materials contain a more extensive list of reference materials.

The grading is based entirely on weekly assignments. For each assignment, you will be asked to write up solutions containing the numerical answers and/or plots where requested, and/or source code which you should put in an SVN repository, which you will learn about in the first week of class.

We do not emphasize the use of computer algebra systems like Mathematica, Maple, or MathCad, but focus more on code development in the C++ language, the programming language in which this course is conducted.

Prior programming experience: It is highly desirable to possess prior programming experience with one or more languages in the "C" family: the most familiar of these are C, C++, Java, PHP, and Perl. If you know C++ already, great, if not we develop the key concepts in object-based C++ programming throughout the course, particularly in the four lecture called *Encapsulation*, *How to write a class,* P*olymorphism and Object Oriented Programming*, and *Templates and the Standard Template Library*.

Students wishing a more elementary primer on more basic elements of C++ (such as datatypes, arrays, structures, control statements, functions) can come to two special lectures outside of the normal meeting time, which we will arrange early in the semester, and/or consult some of the reference materials on reserve in the Engineering library.

Resources: You will obviously need a computer to carry out the assignments in this course. In past years most students have used their personal laptop computer, but if necessary I will put other resources at your disposal. The acceptable computing platforms are linux (which can be installed on a personal computer) or Mac OS machines. During the first week we will strive to make sure every student is set up and able to function on some type of computer. Shortly into the class we will load additional external libraries onto each machine. This "courseware" consists of freely available program libraries plus some custom libraries that I have developed for this course.

This course is in many ways like a laboratory course: while in a laboratory course you build instrumentation and carry out measurements, in this course you will build programs and carry out calculations. *I expect that you will need to interact with me outside of class* for advice on how to do this, particularly because your computing backgrounds vary greatly from student to student. I can provide guidance and advice in program design, debugging, and physics interpretation. My office hours are 1:00-5:00 on Wednesdays but you are welcome to walk into my office whenever you find me there.

Provisional list of reserve materials: The following materials have been placed on reserve in the Engineering Library of Benedum hall. Many of these books are on my shelf if you prefer to stop by and consult them in my office. This list may expand as the semester progresses.

The C programming language, Brian W. Kernighan and Dennis M. Ritchie (1988)

Object-Oriented Analysis and Design with Applications, Grady Booth (1994)

Effective C++ (2005), *More Effective C++,* (1996), and *Effective STL* (2001), Scott Myers

Methods of Numerical Integration, Philip J. Davis and Philip Rabinowitz (1975)

Orthogonal Polynomials, Gabor Szego (1939)

Numerical Methods for Ordinary Differential Equations, J.C. Butcher (2008)

Numerical Recipes: the art of scientific computing, William H. Press et al. (2007)

Modern Quantum Chemistry: introduction to advanced electronic structure Attila Szabo (1989)

Neural networks for pattern recognition, Christopher M. Bishop (1995)

Introduction to Percolation Theory, Dietrich Stauffer (1985)

Students with diabilities: If you have a disability for which you are or may be requesting an accommodation, you are encouraged to contact both your instructor and Disability Resources and Services, 140 William Pitt Union, (412) 648-7890/(412) 383-7355 (lTY), as early as possible in the term. DRS will verify your disability and determine reasonable accommodations for this course