Instructor and Hours

Lectures	:	Mon Wed Fri, 5:00–5:50 pm, 222 NSC
Websites	:	http://ublearns.buffalo.edu/ http://www.physics.buffalo.edu/phy411-506/
Instructor	:	Dr. Richard Gonsalves
Office Hours	:	Tu-Th 11:00–12:00, or by appointment (323 Fronczak Hall)
Phone	:	(716) 645-2017 ext. 191
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Course Description

This course integrates the elements of numerical analysis and computer programming to study a variety of problems in classical, quantum, and statistical physics. The course will review basic numerical operations: root finding, interpolation, matrix inversion, numerical differentiation, and quadrature; and structured and object-oriented programming of basic operations in C++ and Mathematica. Numerical techniques will include solution of linear and nonlinear differential equations of classical and quantum physics, boundary-value and eigenvalue problems, Monte Carlo and stochastic methods, statistical analysis of data, the Fast Fourier Transform, computer algebra, and computer graphics.

Learning Outcomes

After completing the second semester of this course you should have mastered elementary algorithms for basic numerical operations, solution of ordinary differential equations, linear algebra, data analysis and random sequences. You should be able to design correct codes (of a few thousand lines) and to perform simulations of realistic physical systems. You should be able to run your codes, analyze the output, and present your results in a form suitable for scientific publication.

Course Requirements

This course will assume familiarity with classical and quantum mechanics, electrodynamics, and thermal physics at the undergraduate level. Familiarity with a programming language will be helpful, but is not required. If you are not familiar with C++ or Mathematica, you will need to choose one of these languages and learn to use it by understanding and modifying the code examples, which will be explained in detail in lecture.

The required textbook for this course is *Computational Physics*, 2nd Edition, by Giordano and Nakanishi (Pearson Prentice Hall, 2006) ISBN 0-13-146990-8. It is available at the University Bookstore and on reserve at the Library. Chapters 1–7 were covered in Fall 2007. Chapters 8–12 will be covered in Spring 2008. Textbook topics will be supplemented with more advanced computational applications in particle physics and cosmology, condensed matter physics, and biophysics, for which detailed lecture notes will be provided.

A very important online reference for this course will be the *Numerical Recipes* books by Press, Teukolsky, Vetterling, and Flannery. Additional online references on specific topics will be provided in lecture.

You will need access to a computer running a recent version of Windows, Mac OS X, or Linux. All software required for this course is available for free or at a very nominal cost, including Mathematica ($4.95) and Microsoft Visual Studio ($19.95) from UBMicro.

While the PHY 411-506 is intended to be a continuation of PHY 410-505 Fall 2007, the chapters in the textbook are relatively independent of one another. PHY 410-505 is therefore not an absolute prerequisite. If you have not taken PHY 410-505, you should review the Fall course webpage http://www.physics.buffalo.edu/phy410-505/ and make sure you are comfortable with the level of physics material and computational skills required to complete the homework assignments.

Homework Assignments

There will be a homework assignment due each week before 5:00 pm on the due date. Late homework, without a valid excuse, will be penalized at the rate of 20% per day overdue. Graduate students will be given some more

difficult assignments based on graduate-level physics. Your assignment may be hand-written or typeset using a word-processing program. Assignments may be printed and submitted in class, or emailed to me as a PDF file. Only one submission of your complete assignment is allowed. Homework assignments will count for 60% of your final grade.

Semester Project

There will be no final exam for this course. Instead, you will complete a semester project on a topic of your choice (to be approved) in computational physics. This should involve the development of a substantial quantity of code (at least a thousand lines), and a write up of the project in the style of a journal article. Also required is a presentation of the project to the class during the final exam period. The project will count for 30% of your final grade.

Class Participation

Credit counting for 10% will be give for class participation, which may include completing brief pre-class and in-class assignments, and brief in-class progress reports on your semester project.

Letter Grades

An aggregate numerical grade of at least 50% will be required to pass this course. PHY 411 and 506 students will be assigned letter grades on separate curves. In past semesters the cutoff for an A grade has been approximately 85%.

If you maintain a passing average on homework assignments but are unable to complete all assignments and/or the semester project with a valid excuse, you may request an Incomplete (I) grade for the course. Incomplete work must be made up when the course is offered again, and before the default deadline.

Resignation

The last day to drop this course without financial liability is Friday January 18, 2008. The last day to drop this course without an "R" grade is Friday January 25, 2008.

If you find that you are failing the course, or if you wish to withdraw from the course for any reason, you may resign with an "R" grade on or before Friday, March 28, 2008.

Academic Integrity

Academic integrity is a core value underlying all scholarly activity in the Department of Physics. Please review UB policy on academic integrity at http://undergrad-catalog.buffalo.edu/policies/course/integrity.shtml (undergraduates) and http://www.grad.buffalo.edu/policies/academic_integrity.pdf (graduate students).

You are encouraged to discuss class material and assignments with your colleagues. However, you should code and run your simulations yourself, and your homework writeup and semester project must be entirely your own effort. If you copy and/or modify code from any source for your assignments you should acknowledge this with an appropriate citation in your writeup.

Students with Disabilities

If you have a disability, (physical or psychological) and require reasonable accommodations to enable you to participate in this course, such as note takers, readers, or extended time on exams and assignments, please contact the Office of Disability Services, 25 Capen Hall, 645-2608, http://www.student-affairs.buffalo.edu/ods/, and also see me me during the first two weeks of class. ODS will provide you with information and review appropriate arrangements for reasonable accommodations.