

# Syllabus

## PY 502, Computational Physics (Fall 2011)

Instructor: Anders Sandvik

Department of Physics, Boston University

Office: SCI 316, phone: (617) 353-3843, e-mail: sandvik@bu.edu

### Overview

This course provides an introduction to some of the most widely used methods of computational physics, including numerical solutions of differential equations (initial and boundary value problems), molecular dynamics simulations, Monte Carlo simulations, and exact diagonalization of quantum many-body Hamiltonians. In addition to giving the students a basic working knowledge of these particular techniques, the goal is to make them comfortable with scientific computing in general, so that they will be prepared to tackle also other computational problem that they may encounter in the future. The Fortran 90 programming language will be used.

### Prerequisites

The participants should have graduate standing or consent of the instructor. Basic knowledge of the Unix (or Linux) operating system (including use of a text editor) and some understanding of elementary computer programming will be assumed. Extensive prior programming skills are not necessary, however; a brief tutorial on the Fortran 90 language will be given at the beginning of the course. The physics knowledge expected will be at the level typically achieved after the first year of graduate school. Reviews of the relevant physics will be integrated with the discussions of numerical algorithms, and hence also first-year graduate students and advanced undergraduate students can take this course.

### Lecture and office hours

The lectures will be given in CAS 327, Tuesday/Thursday 11 to 12:30. The instructor's office hours are Monday 4-5 PM, Wednesday 3-4 PM.

### Computer access and Friday programming tutorials

CAS 327 is a computer lab with 28 workstations for which the students will be given individual accounts. Some hands-on computer work will be done in class, and the students will have access to the lab also to work on their homework assignments. It is reserved for PY502 Fridays 1-3 PM, when a tutor will also be present to assist and answer questions. The tutors/graders for the course are Ying Tang (yingtang@buphy.bu.edu) and Joel Tenenbaum (jesusina@buphy.bu.edu).

### Course material

There is no required text book for this course. Lecture notes, along with other material, such as homework assignments/solutions and program examples, will be made available on the web-site of the course; [physics.bu.edu/py502](http://physics.bu.edu/py502). In addition, the following texts are recommended reading: *Computational Physics*, by J. M. Thijssen (Cambridge University Press, 2001), *Computational Physics*, by N. J. Giordano and H. Nakanishi (Pearson Prentice hall, 2006), *Fortran 90/95 Explained*, by M. Metcalf and J. Reid (Oxford university Press, 2002), *Fortran 90/95 for Scientists and Engineers*, by S. Chapman (McGraw Hill, 2004), and *Numerical Recipes*, by W. H. Press, S. A. Teukolsky, W. Vetterling, and B. P. Flannery (Cambridge University Press) (there are several versions of this book, with programs written in different languages; any will do for learning the numerical algorithms).

## Schedule

The tentative schedule for the lectures is the following (the numbers refer to weeks): 1) Introduction to Fortran 90, 2) Numerical integration (basic integration schemes, stochastic methods for multi-dimensional integrals), 3-5) Numerical solutions of differential equations (classical equations of motion, studies of systems with chaotic dynamics, eigenstates of the Schrödinger equation, time-evolution of wave-packets in quantum mechanics), 6-7) Molecular dynamics simulations (basic schemes for classical many-particle dynamics), 8-10) Monte Carlo simulations (the Metropolis algorithm for equilibrium statistical mechanics, studies of the phase transition in the Ising model of magnetism, liquids and gases), 11) Optimization using simulated annealing, 12-13) Exact diagonalization of quantum systems (ground state and finite-temperature properties of quantum magnets).

## Homework assignments

Approximately 7 sets of homework problems will be assigned. The students will write computer programs based on computational algorithms discussed in class. These assignments constitute a very important part of the course, since the thinking involved in scientific programming can only be developed through practical work. The assignments must be returned by their stated due dates, unless an extension is granted by the instructor. For late return of assignments, a 10% point deduction will be applied for each late day. All programs should be written in Fortran 90.

The programs as well as a short report discussing the results should be handed in to the grader by the stated due date. The solution programs should be sent as an **attachment** in an e-mail to the address `py502@buphy.bu.edu`. The report, **hardcopy required**, can be handed to the instructor in class or brought to his office any time before the deadline.

Every student is expected to work independently on the assignments. However, discussions with fellow students are allowed, indeed encouraged, as long as they are kept on a general level and do not amount to direct copying of ideas or programming solutions. Technical assistance from the instructor and graders (during Friday tutorials) are allowed, e.g., regarding general programming and computer questions. Although discussions and some degree of cooperation between students is allowed, note that **the material turned in must be independently written**.

## Take-home exam and course grade

There will be a take-home exam in which the students have several days (dates to be announced) to work on a computational project and to write a report on the results. This work must be done by each student completely on her/his own, but all class material (lecture notes, program examples on the web page, etc.) and books (or other sources) on the Fortran 90 programming language and other technicalities (such as graphing tools) may be consulted. The final grade will be based 75% on the homework assignments and 25% on the exam.

## Absence policy

The students are expected to attend all lectures. A valid reason for absence should be communicated in advance to the instructor, if possible. More than 5 unjustified absences will lead to a one-step grade reduction.

## Students' responsibility

Students should know and understand the provisions of the CAS Academic Conduct Code (copies of which are available in room CAS 105) and the BU Code of Student Responsibilities (available on the web at [www.bu.edu/lifebook/university-policies/policies-code.html](http://www.bu.edu/lifebook/university-policies/policies-code.html)). Cases of suspected academic misconduct will be referred to the Dean's office.