Syllabus

PY 502, Computational Physics (Fall 2005)

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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. In addition, visualization of computations/simulations will be discussed as an integral part of the course.

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, Wednesdays and Fridays 11 to 12:30 The instructor’s office hours are Mondays 10:30 AM to 12 noon and Thursdays 2:30 PM to 4 PM.

Computer access
CAS 327 is a computer lab, equipped with 27 computer workstations that can run both the Windows and Linux operating systems. The students will be given accounts on these workstations. Linux will be used. 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.

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/~sandvik/teaching/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),

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, simulations at fixed energy and temperature), 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 8 sets of homework problems will be given throughout the semester. 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. All homework 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 (Ling Wang, office SCI 270, e-mail lingwang@bu.edu) 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 can be handed to the instructor in class, or directly to the grader.

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, grader, and IT staff is allowed, e.g., regarding general programming and computer questions. Although discussions and some degree of cooperation between students is allowed, the material turned in must be independently written.

Exam and grading

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 50% on the homework assignments and 50% on the final 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). Cases of suspected academic misconduct will be referred to the Dean’s office.