Syllabus

PY 502, Computational Physics, Fall 2017

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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) in classical and quantum mechanics, Monte Carlo simulations, and numerical 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 PRB 146, Tuesday/Thursday 11 to 12:30. The instructor’s office hours are Wednesday 11 AM - noon and Thursdays 2 - 3 PM. Tutorials will be held some Fridays 1-2 PM.

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. 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): 1-2) Introduction to Fortran 90, 3) Numerical integration (basic integration schemes, stochastic methods for multi-dimensional integrals), 4-6) 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), 7-9) Monte Carlo simulations (the Metropolis algorithm for equilibrium statistical mechanics, studies of the phase transition in the Ising model of magnetism, cluster algorithms, liquids and gases), 10) Spin glasses, optimization using simulated annealing, 11-13) Quantum spin systems (ground state and finite-temperature properties, quantum annealing).

Homework assignments

6 or 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. To make it easier for the grader, name your program file hwx_name.f90. The report, hardcopy required, can be handed to the instructor in class or brought to his office any time before the deadline, or it can be given 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 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.

Course grade

The grade will be based on the homework assignments.

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 BU’s Academic Conduct Code, available on-line at http://www.bu.edu/academics/policies/academic-conduct-code/

Cases of suspected academic misconduct will be referred to the Dean’s office.