Syllabus

PY 502, Computational Physics, Fall 2023

Instructor: Anders Sandvik
Department of Physics, Boston University
Office: SCI 450A, phone: (617) 353-3843, e-mail: sandvik@bu.edu
Grader: Gabe Schumm, e-mail: gschumm@bu.edu

Overview

This course introduces 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. Beyond providing a basic working knowledge of these particular techniques, the goal is to create the foundations for "computational thinking"—the ability to create models of physical phenomena and devise suitable numerical methods to study their properties. The Julia programming languages will be used—the first few lectures will introduce the language.

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 introduction to Julia 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 SCI B58, Tuesday/Thursday 5 to 6:15 PM. Discussion sections will be in the same room, Fridays, 2:30-3:20 PM. The instructor's office hours are Wednesdays 2-3 PM and Fridays 3:30-4:30 PM.

Course material

There is no required text book for this course. Lecture slides/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), 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 Julia, 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

About 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. It is strongly recommended that the homework programs be written in Julia, but exceptions can be made based on discussions with the instructor and grader.

The programs as well as a short report discussing the results in a clear way (so that someone not taking the course would be able to understand what the purpose is of the work and what the results are) should be submitted online (further instructions will be given) by midnight on the stated due date.

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

After each assignment, the instructor will ask one students to give a brief in-class presentation of the solutions during a discussion meeting.

Course grade

The grade will be based on the homework assignments. Active course participation can be rewarded by a one-step increase in grade in border-line clases (i.e., if the score is already close to the next higher grade).

Absence policy

The students are expected to attend all lectures and discussion meetings. 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.