PHYSICS 580

Computational Physics

Spring 2025

Instructor: Fuqiang Wang

Contact Info: Rm 249 at PHYS, fqwang@purdue.edu

Office Hours: by appointment

Lectures: M&W 1:30-2:20 pm, Rm 234 in PHYS

Lab: F 1:30-3:20 pm, SC G046

Lab TA & Grader: Ishan Deo, ideo@purdue.edu, Office Hour: TBA

<u>Textbook:</u> *Computational Physics*, N. Giordano and H. Nakanishi, Pearson Prentice-Hall (2005). *Book web site (on Prof. Nakanishi's webpage):* http://www.physics.purdue.edu/~hisao/book/

This book is required because readings and exercises will be assigned from it. But you do not have to buy the hardcover (Prentice-Hall) edition or buy it new. Amazon should have a paperback edition that costs much less, and used book sites likely offer the book at reasonable prices too.

<u>Course Homepage:</u> https://purdue.brightspace.com. Course materials such as starter programs and assignments will primarily be posted there.

<u>Course Description:</u> This course will introduce students to a variety of problems in physics which can be best tackled using computational techniques. Most of the time very simple numerical methods and computational algorithms will be involved, but some exposure to more complex computing will also be attempted. The primary goal is to teach **computer-based problem solving in physics** – a skill that most physicists find essential these days.

The course is aimed at advanced undergraduates as well as graduate students at any stage. It satisfies the advanced lab requirement for undergraduate physics majors and the lab requirement for the MS degree for physics graduate students.

Co-/Pre-requisites: A physics background in mechanics at the level of PHYS 310 or 410, and quantum mechanics at the level of PHYS 342 (or higher) is required. Background in thermal and statistical physics at the level of PHYS 515 or 416 will be highly beneficial. Practical programming experience is almost essential, although a formal computer science course such as CS 158/159 (or similar) is tolerated as a substitute. This is NOT a programming language course, so you must either be able to write programs already in some language, or else be willing to give yourself a crash course in a suitable language during the first few weeks. Both text and lectures are algorithm-oriented, i.e., not tied to a specific language. However, starter programs and most sample programs will be provided (likely mostly in Python). The problem-solving techniques and algorithms learned in this course should be useful in future work with any programming language.

Assignments and Exams:

Survey: You are asked to fill out the short survey posted on the course website. Doing so before Lecture 3 will give you 10 bonus points toward the course total.

Homework: There will be **seven (7) homework assignments**, roughly one set every 2 weeks. Assignments must be submitted online on Brightspace in PDF form (+ ASCII source code files). Generally, NO LATE HOMEWORK WILL BE ACCEPTED. Homework submissions must always contain a brief discussion of physics – so even if there is no explicit directive in a problem, you must still present the physics your program is addressing. Homework must also include: i) source codes (at least key parts thereof), ii) a

discussion of what your program does and how it does it, iii) graphical outputs illustrating the results, and iv) a description of the nature of numerical approximations used and how such approximations with your specific parameters are adequate for the problem at hand.

Labs: there will be 13 lab assignments, one per week (excluding Week #1). Laboratory activities may take the whole or a portion of the assigned 2-hour lab session. Assignments will be posted in advance for each lab, and you will typically need to complete and hand in a report with required results and information at the start of the following week's lab. In case any task remains unfinished during the allotted lab session, you are encouraged to use the laboratory facilities available for individual usage as well as your own computing resources to complete it.

Labs are an integral component of the course and attendance is mandatory. Excuses can be granted only under special circumstances and by the instructor. In any case, you need to submit all 13 lab reports by their respective due dates.

Exams: There will be NO exams in this course.

Grading: 53% from homeworks (290 points), 47% from labs (260).

Collaborations and Academic Honesty:

We encourage you to share your ideas and knowledge and work together. However, all assignments will be attributed to individual students, so you must limit your collaboration to the exchange of ideas and knowledge (with the only exception being the labs, see below). Copying of any code or reports or any parts thereof is strictly prohibited and will be sanctioned appropriately together with other violations of academic honesty. For the labs only, you may pair up with one other student to do the work, but each of you then must write and submit reports separately, clearly stating who your partner was and what the contributions of each of you were. Pairing need not be permanent but changing pairs frequently is not advised.

References: the books below may be relevant to our subject and useful for reference:

- 1. **H. Golud and J. Tobochnik**, *Introduction to Computer Simulation Methods*, *3rd Ed.*, Addison-Wesley, 2006.
- 2. **R. H. Landau and M. J. Paez**, Computational Physics: Problem Solving with Computers, 2nd edition, Wiley-VCH, 2007.
- 3. **A. Garcia**, Numerical Methods for Physicists, 2nd edition, Prentis-Hall, 1999.
- 4. **D. Knuth**, *The Art of Computer Programming*, Addison-Wesley, 1969.
- 5. W. H. Press et al. Numerical Recipes. 3rd edition. Cambridge, 2007.
- 6. **D. Stauffer**, Annual Reviews of Computational Physics, World Scientific, 1994-2000.

Campus Emergency Notice

In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances. Information about changes to the course will be posted in the Announcements section for each course website.