Computational Physics / PHYS-GA 2000

This course teaches computational physics for physics PhD students. Classes meet Tuesday and Thursday 9:30am to 10:45am, in Room 208 of 194 Mercer.

The textbook is *Computational Physics*, by Mark Newman. I will draw material also from *Computational Physics*, by Philipp Scherer. Not a lot of creativity in book titles in this field. Other resources are:

- Python Data Science Handbook (PDSH) by Jake Van Der Plas.
- Numerical Recipes, by Press, Teukolsky, Vetterling, and Flannery. This book is mostly useful for its insight and not for its code.

If you have never programmed in Python before then Chapter 2 of the book will require your special attention. There are also many online resources for learning the basics of Python. I can recommend Software Carpentry and also Prof. David Pine's *Introduction to Python for science and engineering*, available online through Bobst Library.

Prof. Blanton's office is Room 941 of 726 Broadway, and his email is blanton@nyu.edu. You can come to ask questions about computational physics (or any other subject!) on Tuesdays 11:00am to 12:15pm, or by appointment.

The teaching assistant is Valentino Foit (foit@nyu.edu) Recitation is Friday, 11am-12:15pm, in Room 1045 of 726 Broadway. This time will primarily consist of working on homework assignments.

The class will be participatory. Please read the assignments *before* attending class; you will be expected at certain points to follow along with calculations on your computer.

There will be no exams in this course, but there will be a pretty heavy load of assignments:

- Weekly homeworks: You may consult with each other about the homeworks, but you must write your own individual code and report.
- Semester project: Performed in groups of two or three students each. I have deadlines for two intermediate drafts of this project; the projects are designed such that you will be able to complete them in stages over the semester based on material previously covered in class. The project culminates in a written report and a presentation in December.

All material handed in will consist of reports written in IATEX (the physics standard typesetting system) and as documented Python code which the TA and professor will be able to run to produce the data and plots. You will receive rather specific templates and instructions about code standards to follow!

It is common now for many people to make use of generative AI tools (e.g. Co-Pilot) for programming or other tasks. If you do so in the homeworks or the project, I require you to document doing so, providing the prompt and the raw output. More generally, just remember that these tools are only useful if you can determine that they are working correctly, so using them doesn't save you from checking the results. I do not think there is any reliable evidence right now that they save significant time.

Grades are based on problem sets (65%), the large project and presentation (25%), and class participation (10%).

The classes will proceed as follows (subject to revision!).

| Date | Topic | Reading | Problem Sets |
|----------------|-----------------------------|---------------|----------------------|
| 2024-09-03 (T) | Numbers on computers | Ch. 1, 2, 3 | |
| 2024-09-05 (R) | Arrays & Numerics | PDSH, Ch. 4 | |
| 2024-09-10 (T) | Random Numbers | Ch. 10.1–10.2 | PS#1 |
| 2024-09-12 (R) | Interpolation | Ch. 5.1–5.2 | |
| 2024-09-17 (T) | Integration | Ch. 5.3–5.4 | PS#2 |
| 2024-09-19 (R) | Integration | Ch. 5.5–5.9 | Teams Determined |
| 2024-09-24 (T) | Differentiation | Ch. 5.10–5.11 | PS#3 |
| 2024-09-26 (R) | Differentiation | | |
| 2024-10-01 (T) | Linear Algebra | Ch. 6.1 | PS#4 |
| 2024-10-03 (R) | Linear Algebra | Ch. 6.1 | |
| 2024-10-08 (T) | Eigensystems | | PS#5 |
| 2024-10-10 (R) | Eigensystems | Ch. 6.2 | |
| 2024-10-15 (T) | Legislative Monday—no class | Ch. 6.2 | PS#6 |
| 2024-10-17 (R) | Root-finding | Ch. 6.3 | |
| 2024-10-22 (T) | Minimization | Ch. 6.4 | Project draft #1 due |
| 2024-10-24 (R) | Minimization | Ch. 6.4 | |
| 2024-10-29 (T) | Minimization | Ch. 6.4 | PS#7 |
| 2024-10-31 (R) | Fourier Analysis | Ch. 7 | |
| 2024-11-05 (T) | Ordinary DEs | Ch. 8.1–8.3 | PS#8 |
| 2024-11-07 (R) | Ordinary DEs | Ch. 8.4–8.5 | |
| 2024-11-12 (T) | Ordinary DEs | Ch. 8.6 | |
| 2024-11-14 (R) | Partial DEs | Ch. 9.1 | |
| 2024-11-19 (T) | Partial DEs | Ch. 9.2 | Project draft #2 due |
| 2024-11-21 (R) | Partial DEs | Ch. 9.3 | |
| 2024-11-26 (T) | Partial DEs | Ch. 9.3 | PS#9 |
| 2024-11-28 (R) | Thanksgiving, no class | | |
| 2024-12-03 (T) | Markov Chain Monte Carlo | _ | |
| 2024-12-05 (R) | Gaussian Processes | _ | |
| 2024-12-10 (T) | Gaussian Processes | _ | PS#10 |
| 2024-12-12 (R) | Using GPUs | _ | Final project due |
| Exam week | Project presentations | _ | |