UNIVERSITY of HOUSTON

DEPARTMENT OF PHYSICS

Physics 6350 Computational Physics Spring 2025

Lecture: TuTh 10:00 AM – 11:30 AM
Lab: TH 9:00 AM – 10:00 AM

Professor Volodymyr Vovchenko, email: vvovchenko@uh.edu

Office Hours: Wednesday 11AM-1PM or by appointment (office SR1 629C)

(Last update 5/1/2025)

Catalog Description
Simulation of classical and quantum mechanical problems on digital computers using numerical and modern programming techniques.

Topics to be covered
General introduction to scientific programming and visualization. Numerical methods in linear algebra. Numerical integration and differentiation. Numerical solutions to ordinary and partial differential equations, and to systems of non-linear equations. Molecular dynamics and Monte Carlo simulations. Problems from classical, statistical, and quantum mechanics. Data processing and curve fitting. Introduction to parallel computing.

Course Requirements
It is essential that everyone has an account on a machine where you can write, compile, and run code either in Python (Jupyter notebook preferred) or C/C++, both during and outside of lecture. You may work in whatever operating system you prefer.

Coursework

A. **Lectures**: Attendance at lectures is required. Excused absences will be allowed for appropriate situations; see the Excused Absence Policy below. Lectures notes and example code will be posted before class.
B. **Exams**: There will be two exams, a midterm and a final. The exams may consist of multiple choice, short answer, and/or long answer problems to show your understanding of the techniques we cover. The final is likely to include some quick programming exercises.
C. **Homework**: Homework assignments will be given every 1-2 weeks. Each assignment is worth 12 points, the instructor will drop the lowest scoring homework.
D. **Final Project**: Each student will complete a project on a pre-approved topic, due on the last day of class. Group projects are possible but require prior approval.

Grades
The coursework will be given the following weights when calculating the semester grade:
Homework: 40%
Final Project: 20%
Midterm Exam: 15%

Final Exam: 25%

Bonus points

- Fill out course evaluation survey (2 points)
- On an individual basis where warranted

Grading scale

Your grade will be determined by your total number of points (out of 100)

Total Points	**Grade**
90-100	A
85-89.99	A-
80-84.99	B+
70-79.99	B
60-69.99	B-
55-59.99	C+
50-54.99	C
45-49.99	C-
40-44.99	D+
35-39.99	D
30-34.99	D-
0-29.99	F

Lecture Slides and Example Code

https://github.com/vlvovch/PHYS6350-ComputationalPhysics

Textbooks

There is no assigned textbook. Some material overlaps with the following textbook:

- *Computational Physics* by Mark Newman (Some parts of this text are available on the author's website: http://www-personal.umich.edu/~mejn/cp/index.html)

The following textbooks can be also useful:

- *Numerical Recipes: The Art of Scientific Computing,* Third Edition by W.H. Press, et al.,
- *Computational Physics*, 2nd edition, by Giordano and Nakanishi
- *Introduction to Computational Physics,* by Richard Fitzpatrick (Available online at https://farside.ph.utexas.edu/teaching/329/329.html)

Tentative Schedule (Last update 4/24/2025)

1/14	Introduction, Syllabus, Technical Details
1/16	Visualization of Data, Machine Precision
1/21	No lecture (snow)
1/23	Function Interpolation
1/28, 1/30	Linear Algebra and Matrices
2/4, 2/6	Nonlinear Equations
2/11, 2/13, 2/18	Numerical Calculus
2/20, 2/25	Numerical Differential Equations
2/27	Problems in Classical Mechanics
3/4	Molecular Dynamics
3/6	Midterm Exam
3/11, 3/13	Spring Break – no classes
3/18, 3/20, 3/25	Partial Differential Equations
3/27, 4/1	Random Numbers and Monte Carlo Methods
4/3	Problems in Statistical Physics
4/10	Intro to Machine Learning
4/15	Problems in Statistical Physics
4/17	Problems in Quantum Mechanics
4/22	Final Project Presentations
4/24	Final Project Presentations, Review
5/6, 10am-12pm	Final Exam

Homework: Every 1-2 weeks, due on Friday the following week
Final Projects: Due on the last day of class, 4/24.

Excused Absence Policy
Excused absences from lecture will be granted for appropriate reasons, which include, but are not limited to, medical issues, caretaking responsibilities, university sponsored activities, emergencies, etc. If you are going to miss lecture and want your absence to be excused, you must notify me in writing (email is fine) prior to the absence if possible, or as soon as possible after the absence with an explanation as to why the notice could not be sent before the absence. You may be required to provide documentation to support the reason for the absence. You will be required to make up any course work missed due to the absence. The same policy applies to requests to extend assignment due dates. See also the University Excused Absence Policy below.

AI Tools: The use of Artificial Intelligence tools such as ChatGPT is permitted for troubleshooting/assistance purposes but should not be relied upon. The student should be able to explain what their code does in full upon request from the instructor

Standard Disclaimer: This syllabus is subject to change at the discretion of the instructor.

Addendum: Whenever possible, and in accordance with 504/ADA guidelines, the University of Houston will attempt to provide reasonable academic accommodations to students who request and require them. Please call 713-743-5400 for more assistance.

Academic Honesty: It is each student's responsibility to read and understand the Academic Honesty Policy found at http://catalog.uh.edu/content.php?catoid=34&navoid=12627.

Religious Holy Days: Students whose religious beliefs prohibit class attendance or the completion of specific assignments on designated dates may obtain an excused absence. To do so, please make a written request for an excused absence and submit it to your instructor as soon as possible, to allow the instructor to make arrangements. See http://publications.uh.edu/content.php?catoid=36&navoid=12931.

Counseling and Psychological Services (CAPS) can help students who are having difficulties managing stress, adjusting to college, or feeling sad and hopeless. You can reach CAPS (http://www.uh.edu/caps) by calling 713-743-5454 during and after business hours for routine appointments or if you or someone you know is in crisis. Also, there is no appointment necessary for the "Let's Talk" program, which is a drop-in consultation service at convenient locations and hours around campus. https://uh.edu/caps/outreach/lets-talk

University Excused Absence Policy:
Regular class attendance, participation, and engagement in coursework are important contributors to student success. Absences may be excused as provided in the University of Houston Undergraduate Excused Absence Policy and Graduate Excused Absence Policy for reasons including: medical illness of student or close relative, death of a close family member, legal or government proceeding that a student is obligated to attend, recognized professional and educational activities where the student is presenting, and University-sponsored activity or athletic competition. Additional policies address absences related to military service, religious holy days, pregnancy and related conditions, and disability.

Recording of Class
Students may not record all or part of class, livestream all or part of class, or make/distribute screen captures, without advanced written consent of the instructor. If you have or think you may have a disability such that you need to record class-related activities, please contact the Center for Students with DisABILITIES. If you have an accommodation to record class-related activities, those recordings may not be shared with any other student, whether in this course or not, or with any other person or on any other platform. Classes may be recorded by the instructor. Students may use instructor's recordings for their own studying and notetaking. Instructor's recordings are not authorized to be shared with *anyone* without the prior written approval of the instructor. Failure to comply with requirements regarding recordings will result in a disciplinary referral to the Dean of Students Office and may result in disciplinary action.

Syllabus Changes
The instructor may need to make modifications to the course syllabus and may do so at any time. Notice of such changes will be announced as quickly as possible.