UCONN
UNIVERSITY OF CONNECTICUT

Department of Physics
College of Liberal Arts & Sciences

PHYS 5350 – Introduction to Computational Physics

Course Syllabus, Fall 2022

Syllabus information is subject to change. The most up-to-date syllabus is located within the course in HuskyCT.

Instructor and Course Information

Prof. Daniel Anglés-Alcázar

E-mail: angles-alcazar@uconn.edu
Class meetings: Mondays/Wednesdays at 12:30PM - 1:45PM
Class location: GS 119
Office hours: Mondays at 5:00PM - 6:00PM in Gant South S113G, or by appointment.
Online by appointment: https://uconn-cmr.webex.com/join/daa19013

Course Description

Description: Broad introduction to methods in computational physics, including Python programming and applications in a supercomputing environment.

Goals:

1. To understand the basic principles of numerical algorithms to solve a variety of problems in Physics and the limitations of numerical methods.
2. To become proficient in computer programming using Python and gain experience writing code to solve current problems.
3. To explore the structure and functioning of modern supercomputing centers and learn the basics of high-performance computing.
4. To develop data presentation and scientific writing skills required to produce competitive proposals to use national supercomputing facilities in your research.

Course Structure and Class Dynamics:

- Reading assignments will be completed prior to discussing each topic in class.
- The course materials will be presented through a mix of short overview lectures and discussion of interactive examples.

- A significant portion of class time will be devoted to individual and group work on coding exercises, using your personal laptop computer, and based on the reading assignment and lecture materials.
- During the semester, you will complete a total of six homework assignments building on class exercises.
- A final project consisting of a written supercomputing proposal and a related oral presentation will be required.

Course Materials

Required textbook: Computational Physics, Mark Newman, 2012. ISBN-13: 978-1480145511. It should be available in the UConn Bookstore. (see also Amazon Link). Many reading assignments will be based on this textbook, and so this is a required course material. Lecture notes and links to additional online materials will be provided through HuskyCT.

Laptop computer: Access to a laptop computer will be required to complete the coding exercises during class time, the homework assignments, and the final project. Please, let me know if you do not have access to a suitable laptop computer so that we can discuss options as soon as possible.

Python: We will use the Python programming language throughout this course. You should have a working Python installation in your laptop (see e.g. the Anaconda Python distribution). We will also develop and run Python code remotely in a supercomputing center. See some excellent Python tutorials at:
https://github.com/jakevdp/WhirlwindTourOfPython by Jake Vanderplas.
https://github.com/jakevdp/PythonDataScienceHandbook by Jake Vanderplas.
https://github.com/jrjohansson/scientific-python-lectures by Robert Johansson.

LaTeX: The written proposal will be submitted as a PDF document created in LaTeX. You can open an account and run LaTeX online at https://www.overleaf.com. Alternatively, you should feel free to install LaTeX in your computer. If you are new to LaTeX, you can find very good tutorials at https://www.overleaf.com/learn.

Expectations

General Rules of Conduct: Everyone is expected to contribute to a respectful, welcoming, and inclusive environment. Every member of this course is required to embrace the diversity of this class, including academic level, age, background, gender identity and expression, ethnicity, national origin, religious affiliation, sexual orientation, and other visible and non-visible categories. Bullying, harassment, or discrimination of

any type between members of this course will not be tolerated. Please, do your best to make everyone feel safe and welcome in class!

Electronic devices: The use of laptops in class is restricted to take notes, work on class exercises, etc. Make sure to silence your cellphone when entering class and refrain from using your cellphone/tablet/laptop for anything other than class work. You may be asked to leave class for repeated distractions caused by electronic devices.

Academic Integrity: Group work is accepted and encouraged for the homework and project assignments. Discussing Python problems with classmates and learning from each other is fine, but simply copying someone else's work (either code or text) or letting someone copy yours is cheating. The failure to adequately document the source(s) used in your work is plagiarism, and it is also against the UConn Student Code (http://community.uconn.edu/the-student-code-preamble). If you are found to be cheating in any way, the incident will be reported to Academic Misconduct.

COVID: Review UConn policies on COVID at https://covid.uconn.edu.
While masks are not required indoors (except for a few exceptions), I encourage everyone to wear mask in class. In either case, we are all expected to respect each other's decisions and comfort level with masking and COVID. Please, stay home and do not come to class if not feeling well, particularly in the case of having covid-like symptoms. Refer to SHaW for instruction on the requirements of self-isolation and self-quarantine: https://studenthealth.uconn.edu/updates-events/coronavirus. If you miss class (for whatever reason), (1) check in with a colleague to find what you missed, (2) read over the content in the textbook, assigned pre-class readings, and class notes posted on HuskyCT, and (3) ask any questions that you have!

Please, remember that everyone is experiencing their own unique challenges right now and we may all use some help to get moving forward.

How to Succeed in this Course

General suggestions for how to succeed in this course:

- Attend class and read any assigned materials before class.
- Review the examples after class and make sure that you understand everything.
- Ask questions anytime during the class.
- Plan ahead and start working on the homework assignments and final proposal early. Don't wait until the last minute!
- Come to office hours to discuss any aspect of this class.

Please let me know as soon as possible if there is anything that prevents you from learning and making progress in this class. We all need accommodations because we all

learn differently, and we will develop strategies to meet both your needs and the course requirements. The number one priority is always the physical, mental, and emotional well-being of everyone. Course policies can be adapted for students on a case-by-case basis if required due to extenuating circumstances.

Course Schedule

This is the tentative schedule for the semester (subject to change depending on the time spent on each topic according to the interest and participation level of the class):

Week	Dates	Topic	Reading Assignment	Notes
1	Aug 29 - 31	Syllabus, Python overview	2	
2	Sept 5 - 7	Unix command line, Supercomputing environment	Class notes	No class Sep 5 HW #1
3	Sept 12 - 14	Visualization, Accuracy	3, 4	
4	Sept 19 - 21	Integrals and derivatives	5	HW #2
5	Sept 26 - 28	Parallel computing		Guest lectures
6	Oct 3 - 5	Linear and non-linear equations	6	HW #3
7	Oct 10 - 12	Fourier transforms	7	
8	Oct 17 - 19	Ordinary differential equations	8	HW #4
9	Oct 24 - 26	Partial differential equations	9	
10	Oct 31 - Nov 2	Partial differential equations	9	HW #5
11	Nov 7 - 9	Monte Carlo methods	10	
12	Nov 14 - 16	Machine Learning	Class notes	Proposal abstract
13	Nov 21 - 23	**Thanksgiving Recess**		
14	Nov 28 - 30	Machine Learning	Class notes	HW #6
15	Dec 5 - 7	Proposal presentations		
16	Dec 12 - 14	**Final exams week**		Written proposal

Course Grading

The final course grade will be based on class work, homework assignments, an oral presentation, and a written proposal according to the following weights:

Grade Component	Weight
Class work	**10%**
Homework assignments	**60%**

Proposal presentation	**10%**
Written proposal	**20%**

Grading Scale (%)			
93-100 A	83-86 B	73-76 C	63-66 D
90-92 A-	80-82 B-	70-72 C-	60-62 D-
87-89 B+	77-79 C+	67-69 D+	0-59 F

Participation: You are expected to follow the rules of conduct, participate in class, and contribute to the overall functioning of the course.

Class work: The coding exercises during class time represent 10% of the final grade.

Homework assignments: Each computational physics problem will be evaluated according to best programming practices, the numerical methods employed, and the solution provided. Six homework assignments will account for 60% of the final grade.

Final proposal: The written supercomputing proposal (20% of the final grade) will follow the format required by XSEDE (https://www.xsede.org) (now replaced by ACCESS), including an introduction to the necessary scientific background, description of computational methods, demonstration of code capabilities, and justification of computational resources requested. You are free to choose a computational problem of your interest, but the proposed code should make efficient use of high-performance computing resources. Oral presentations describing the proposed work will account for 10% of the final grade. Groups of up to two students per project are allowed.

UConn Policies

Policy Against Discrimination, Harassment and Related Interpersonal Violence

The University is committed to maintaining an environment free of discrimination or discriminatory harassment directed toward any person or group within its community – students, employees, or visitors. Academic and professional excellence can flourish only when each member of our community is assured an atmosphere of mutual respect. All members of the University community are responsible for the maintenance of an academic and work environment in which people are free to learn and work without fear of discrimination or discriminatory harassment. In addition, inappropriate amorous relationships can undermine the University's mission when those in positions of authority abuse or appear to abuse their authority. To that end, and in accordance with federal and state law, the University prohibits discrimination and discriminatory harassment, as well as inappropriate amorous relationships, and such behavior will be met with appropriate disciplinary action, up to and including dismissal from the University. Additionally, to protect the campus community, all non-confidential University employees (including faculty) are required to report sexual assaults, intimate partner violence, and/or stalking involving a student that they witness or are told about to the Office of Institutional Equity. The University takes all reports with the utmost

seriousness. Please be aware that while the information you provide will remain private, it will not be confidential and will be shared with University officials who can help. More information is available at equity.uconn.edu and titleix.uconn.edu.

Religious Observances and Extra-Curricular Activities

Faculty and instructors are expected to reasonably accommodate individual religious practices unless doing so would result in fundamental alteration of class objectives or undue hardship to the University's legitimate business purposes. Such accommodations may include rescheduling an exam or giving a make-up exam, allowing a presentation to be made on a different date or assigning the student appropriate make-up work that is intrinsically no more difficult than the original assignment. Faculty and instructors are strongly encouraged to allow students to complete work missed due to participation in extra-curricular activities that enrich their experience, support their scholarly development, and benefit the university community. Examples include participation in scholarly presentations, performing arts, and intercollegiate sports, when the participation is at the request of, or coordinated by, a University official. Students should be encouraged to review the course syllabus at the beginning of the semester for potential conflicts and promptly notify their instructor of any anticipated accommodation needs. Students are responsible for making arrangements in advance to make up missed work.

For conflicts with final examinations, students should contact the Dean of Students Office. Faculty and instructors are also encouraged to respond when the Counseling Program for Intercollegiate Athletes (CPIA) requests student progress reports. This will enable the counselors to give our students appropriate advice.

Students with Disabilities

The University of Connecticut is committed to protecting the rights of individuals with disabilities and assuring that the learning environment is accessible. If you anticipate or experience physical or academic barriers based on disability or pregnancy, please let me know immediately so that we can discuss options. Students who require accommodations should contact the Center for Students with Disabilities, Wilbur Cross Building Room 204, (860) 486-2020 or http://csd.uconn.edu

Emergency Management on Emergency Preparedness

In case of inclement weather, a natural disaster, or a campus emergency, the University communicates through email and text message. Students are encouraged to sign up for alerts through http://alert.uconn.edu. Students should be aware of emergency procedures, and further information is available through the Office of Emergency Management at http://publicsafety.uconn.edu/emergency