

Syllabus for PHYS 6350: Computational Physics.

Prof G Morrison

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Fall 2020

MWF 9-10am, Science & Research 1 Rm 606

W 10-11am, Science & Research 1 Rm 606

Office Hours: Monday 10am-11am, Wednesday 11am-12pm, Friday 10am-11am

An appointment is required if you would like to speak outside of office hours

This course is a HyFlex course. Some students may have a designated face-to-face spot reserved, but alternative ways to participate will also be provided. These alternatives may include (but are not limited to) attending class sessions through synchronous streaming, viewing recordings of class meetings asynchronously, participating in discussion boards, and/or completing self-directed activities. This course will have a final exam per the [University schedule](#). As the University will be transitioning all classes and final exams given after the Thanksgiving Break to online delivery, the exam for this course will be delivered in the synchronous online format, and the specified date and time will be announced during the course. Prior to the exam, descriptive information, such as the number and types of exam questions, resources and collaborations that are allowed and disallowed in the process of completing the exam, and procedures to follow if connectivity or other resource obstacles are encountered during the exam period, may be provided.

Livestreaming of the lecture will be conducted in MS Teams. You will receive link to join the Team prior to the first day of class or upon joining either the in-person or online course. If you are registered in the online section, you are not permitted to join the course in-person, and may be refused access to the room. Social distancing is not possible if a crowd develops outside of the classroom, so please do not attempt to join the face-to-face class without permission.

Please note that there will be *absolutely no penalty* for a student registered for the in-person section choosing to join the class online, *so long as they do join the synchronous class online*. This is true for any reason: e.g. if you wake up late you can just join online. You do not need prior permission attend the class virtually, and I will never ask you the reason you chose to attend the class online on any particular day. This very flexible policy exists to ensure that each student is comfortable with the following very important requirement:

If a face-to-face student feels at all sick or feels concerned they have been in close contact with a Covid-positive person, they should stay home and join the class online. This is consistent with university policy, described below. Attendance will still be collected every day, but no differentiation will be made for in-person vs. online attendance. You do not need to provide advanced notice, nor do you need a doctor's note, to miss the in-person section *as long as you join the lecture online.*

Additional details about university policy regarding HyFlex courses and preventing the spread of COVID-19 can be found at the end of the syllabus. Please read these details carefully, as you will be expected to follow university rules and may be removed from class if you are in violation of any policy.

Required Textbook: Alejandro Garcia's *Numerical Methods for Physics* and/or Alejandro Garcia's *Numerical Methods for Physics (Python)*. Note that these books are relatively inexpensive (<\$20 each). A familiarity with both C++ and Python will be required for the course. Material from other textbooks or the recent literature may be used in lecture (and will be posted to Teams if so) or in homework

- Other materials will be used in lectures as well. In particular, Hartmann and Rieger's "A Practical Guide to Computer Simulations" (<https://arxiv.org/abs/cond-mat/0111531v1>) will be discussed early in the course, and will be posted to the Teams Page. Later in the course, special topics will largely be drawn from the recent literature.
- Lecture will blend theory and computational topics, and you will be expected to be able to perform theoretical calculations as well as simulations. You are encouraged (but are not required) to bring your laptop to class if we are going to discuss code. The focus of each lecture will be announced at the end of the preceding class period.

Grading Structure: Your final grade will be determined by

- Homework: 40%. Homework will be assigned weekly, except the week on which the midterm occurs.
- Final exam: 30%. Your final exam will be open-book, open-note, open-internet in early December.
- Midterm exam: 15%. There will be one midterm exam, open-book, open-note, open-internet in mid-October.
- Attendance: 10%. Due to the hybrid nature of the course, attendance must be taken every day. This will be in the form of a poll related to the lecture that you will have ~ 1 minute to answer, at a random time during the lecture.
- Github use: 5%. In addition to posting your homework and exam solutions to Teams, you will receive additional credit for uploading your code to Github. The code you post must be commented, and have a description of the purpose of the code.

Expected schedule of topics. The timing of each topic may vary throughout the semester without prior warning. Weeks with a mark denote administrative events or holidays.

Week	Dates	Topic
1	Aug 24-28	Introduction to programming
2*	Aug 31- Sep 4	Practical Approaches to Programming
3**	Sept 9-11	Numerical solutions to ODEs (Garcia Ch 2-3)
4	Sept 14-18	Numerical solutions to ODEs (Garcia Ch 3)
5	Sept 21-25	Numerical Matrix Methods (Garcia Ch 4, 9)
6	Sept 28-Oct 2	PDEs (PDEs Garcia Ch 6)
7	Oct 5-9	PDEs (Garcia Ch 7, 9)
8	Oct 12-16	PDEs (Garcia Ch 7-8)
9	Oct 19-23	Monte Carlo Integration (Garcia Ch 9)
10	Oct 26-30	MCMC & Gillespie (notes)
11†	Nov 2-6	Molecular Dynamics (Garcia Ch 11, notes)
12	Nov 9-13	Special Topics
13‡	Nov 23	Special Topics
14	Nov 30-Dec 4	Special Topics

*: Last day to add a class, Aug 31. **: Labor day, Sept 7. † Last day to drop with a W, Nov 3. ‡: Thanksgiving Break, Nov 25-27.

If topics from weeks 1-11 take longer than expected, these topics will be discussed in weeks 12-14 as needed. If possible special topics may include: Principal Component Analysis, Machine Learning/Tensor Flow, PageRank and Centrality in Networks, Quantum Computing, Replica Exchange Methods, Weighted Histogram Methods, Lattice Boltzmann Techniques.

Face Covering Policy

To reduce the spread of COVID-19, the University [requires face coverings](#) on campus including classrooms for both faculty and students. Face coverings must cover your mouth and nose and be worn throughout the class session. A mask with a valve is not considered an adequate face covering and should not be used, as it can expel exhaled air, increasing the risk to others. Eating or drinking during class is discouraged and is not an excuse for removing the face covering for any extended length of time. For additional information on the use of face coverings, please see [Face Covering FAQs](#). Failure to comply with the requirement to wear a face covering in class will result in your being asked to leave the classroom immediately and a disciplinary referral through the Dean of Students Office. Requests for accommodations relating to the face covering policy may be directed to the [Center for Students with DisABILITIES \(CSD\)](#).

Required Daily Health Self-Assessment

Your presence in class each session means that you have completed a daily self-assessment of your health/exposure and you:

- Are NOT exhibiting any [Coronavirus Symptoms](#)
- Have NOT tested positive for COVID-19
- Have NOT knowingly been exposed to someone with COVID-19 or suspected/presumed COVID-19

If you are experiencing any COVID-19 symptoms that are not clearly related to a pre-existing medical condition, do not come to class. Please see [COVID-19 Diagnosis/Symptoms Protocols](#) for what to do if you experience symptoms and [Potential Exposure to Coronavirus](#) for what to do if you have potentially been exposed to COVID-19. Consult the (select: [Undergraduate Excused Absence Policy](#) or [Graduate Excused Absence Policy](#)) for information regarding excused absences due to medical reasons.

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

Due to the changing nature of the COVID-19 pandemic, please note that 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 through email and MS Teams.

Resources for Online Learning

The University of Houston is committed to student success, and provides information to optimize the online learning experience through our [Power-On](#) website. Please visit this website for a comprehensive set of resources, tools, and tips including: obtaining access to the internet, AccessUH, and Blackboard; requesting a laptop through the Laptop Loaner Program; using your smartphone as a webcam; and downloading Microsoft Office 365 at no cost. For questions or assistance contact UHOnline@uh.edu.

UH Email

Email communications related to this course will be sent to your [Exchange email account](#) which each University of Houston student receives. The Exchange mail server can be accessed via Outlook, which provides a single location for organizing and managing day-to-day information, from email and calendars to contacts and task lists. Exchange email accounts can be accessed by logging into Office 365 with your CougarNet credentials or through Access UH. They can also be configured on [iOS](#) and [Android](#) mobile devices. Additional assistance can be found at the [Get Help](#) page.

Webcams

Access to a webcam is required for students participating remotely in this course. During lecture, webcam use is not required at any point during the class. If you wish to attend office hours remotely, you must turn on your webcam to promote ease of conversation.

Honor Code Statement

Students may be asked to sign an honor code statement as part of their submission of any graded work including but not limited to projects, quizzes, and exams: *"I understand and agree to abide by the provisions in the [University of Houston Graduate Academic Honesty Policy](#). I understand that academic honesty is taken very seriously and, in the cases of violations, penalties may include suspension or expulsion from the University of Houston."*

Final Exam

An alternative assessment will be used in the place of the traditional final exam at the course conclusion. Instructions will be provided, including the date and time that the assessment materials will be released to the class and will be due, resources and collaborations that are allowed and disallowed in the process of completing the assessment, procedures to follow if connectivity or other resource obstacles are encountered during the assessment period, acceptable submission formats, and submission location.

Helpful Information

COVID-19 Updates: <https://uh.edu/covid-19/>

Coogs Care: <https://www.uh.edu/dsaes/coogscare/>

Laptop Checkout Requests: <https://www.uh.edu/infotech/about/planning/off-campus/index.php#do-you-need-a-laptop>

Health FAQs: <https://uh.edu/covid-19/faq/health-wellness-prevention-faqs/>

Student Health Center: <https://uh.edu/class/english/lcc/current-students/student-health-center/index.php>