

PHYS220/MATH220 : SCIENTIFIC COMPUTING I

Fall 2019

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Office Hours: By appointment.

Course Page: <https://github.com/chapman-phys220-2020s>

Course Description: This example-driven course introduces computation as a tool for scientific exploration. Topics include manuscript preparation with LaTeX and Jupyter, test-driven development, numerical methods with arrays/dataframes, and symbolic computation. Modern languages like Python, MATLAB, Sage, and Julia are emphasized.

Prerequisites: CPSC230

Course Textbook:

Effective Computation in Physics: Field Guide to Research with Python, Scopatz & Huff, 2015.
<http://physics.codes>

Supplementary Python/SciPy Web Resources:

<http://github.com/chapman-phys220-2019f/info>
<http://www.scipy-lectures.org>
http://lectures.quantecon.org/py/learning_python.html
<http://numba.pydata.org/numba-doc/0.12.2/quickstart.html> (Numba Quickstart)
<https://youtu.be/eK1NEJ1SjuE> (Introduction to Numba)
<https://youtu.be/6oXedk2tGfk> (Numba for Accelerating Scientific Computation)

Grading Policy:

Homework (30%), In-class work (20%), Midterm Project (20%), Final Project (30%).

Organization:

This course is intended to develop a professional skill set aimed at getting jobs related to physics, mathematics, or computer science after college. The tools we will use are not watered down—they are exactly the tools becoming increasingly used in industry and academia for scientific computing and data science. *Practice is essential*. As such, it is your responsibility to arrive prepared to complete the in-class group projects in an efficient and productive manner. You are expected to turn in professional-quality work that is documented according to industry standards. Your work should be bug-free, well-tested, and elegantly written. Half of your job is solving interesting problems; the other half of your job is proudly presenting your results as a professional.

The bulk of in-class time will be spent in groups solving interesting physical problems using a computer. You will put into practice what you have read from the textbook and web resources, with

guidance from the instructor and peers. Homework will be a more challenging extension of what is covered in class to provide additional practice. The midterm and final projects will be more substantial and completed individually. They will require a synthesis of all topics learned in the course to complete successfully.

Laptop:

You will use software installed on your own laptop, and it is your responsibility to manage that software and ensure compatibility with the expectations of the course. The software you need is almost entirely contained in the python distribution *Anaconda* (<http://www.anaconda.com/download>), which includes Python, Numeric Python, Scientific Python, Pandas, Numba, and many other packages. You will also need access to a bash terminal and the `git` program: both are automatically available in Linux or Mac, and can be installed in Windows as part of the *Git for Windows* (<http://git-scm.com/download/win>) application. We will spend the first few classes downloading and installing software so that everyone is on the same page.

GitHub:

Homeworks, classworks, and exams will be assigned and collected on the industry-standard cloud code-sharing site GitHub (<http://www.github.com>), using the `git` change-control tool. You will be expected to create an account and know how to use it. The GitHub Organization for the course will be <http://github.com/chapman-phys220-2020s>.

Slack:

Group discussion and contact with the professor will be facilitated by the industry-standard chat application Slack, at <http://scststudents.slack.com>. Please notify the instructor if you need to be invited. The channel for this course will be `#phys220-2020s` and is set to auto-notify the instructor. Note that the class channel is a public forum, but private chats are also available as needed.

Course Learning Outcomes:

1. Create professional reports in \LaTeX , including proper section structuring, figures, and references. Augment these static reports with dynamic Jupyter notebooks that are targeted for web publication as supplementary information.
2. Demonstrate industry-standard software engineering principles, including modular design, test-driven development, change control (git), and the efficient use of console editors (nano/vim) for code development.
3. Write simulation code involving precision numerical methods and array-based numerical processing in Python and MATLAB, as well as dataframe manipulation and symbolic computation in Python. Demonstrate the use of vectorized code and compiled libraries for efficiency, as well as a familiarity with just-in-time compilation.
4. Produce accurate simulations of challenging physical systems, with the explicit goal of using those simulations to answer interesting scientific questions.

Physics Program Learning Objectives:

Upon graduation:

1. Students will recall and use mathematics to precisely formulate and solve physical problems.
2. Students will recall and use core principles of classical mechanics, electromagnetism, quantum mechanics, thermal physics, and statistical mechanics to model and analyze a variety of physical phenomena.
3. Students will use both laboratory and computational skills to take measurements, numerically simulate physical models, and analyze data to draw valid conclusions.
4. Students will effectively communicate scientific results to both technical and general audiences.
5. Students will demonstrate that they can think critically and work both independently and in collaborative teams.

Chapman University Academic Integrity Policy:

Chapman University is a community of scholars that emphasizes the mutual responsibility of all members to seek knowledge honestly and in good faith. Students are responsible for doing their own work and academic dishonesty of any kind will be subject to sanction by the instructor/administrator and referral to the university Academic Integrity Committee, which may impose additional sanctions including expulsion. Please review the full description of Chapman University's policy on [Academic Integrity](#).

Chapman University Students with Disabilities Policy:

In compliance with ADA guidelines, students who have any condition, either permanent or temporary, that might affect their ability to perform in this class are encouraged to contact the Office of Disability Services. If you will need to utilize your approved accommodations in this class, please follow the proper notification procedure for informing your professor(s). This notification process must occur more than a week before any accommodation can be utilized. Please contact [Disability Services](#) at (714) 516-4520 if you have questions regarding this procedure or for information or to make an appointment to discuss and/or request potential accommodations based on documentation of your disability. Once formal approval of your need for an accommodation has been granted, you are encouraged to talk with your professor(s) about your accommodation options. The granting of any accommodation will not be retroactive and cannot jeopardize the academic standards or integrity of the course.

Chapman University Equity and Diversity Policy:

Chapman University is committed to ensuring equality and valuing diversity. Students and professors are reminded to show respect at all times as outlined in Chapman's [Harassment and Discrimination Policy](#). Please review the full description of Harassment and Discrimination Policy. Any violations of this policy should be discussed with the professor, the Dean of Students and/or otherwise reported in accordance with this policy.

Student Support at Chapman University:

Over the course of the semester, you may experience a range of challenges that interfere with your learning, such as problems with friend, family, and or significant other relationships; substance use; concerns about personal adequacy; feeling overwhelmed; or feeling sad or anxious without knowing why. These mental health concerns or stressful events may diminish your academic performance and/or reduce your ability to participate in daily activities. You can learn more about the resources available through Chapman University's [Student Psychological Counseling Services](#).

Approximate Course Outline:

Week	Tuesday	Thursday	Topics
1	Orientation	Read: Ch. 1	bash , remote access
2	Read: Ch. 15	Read: Ch. 16	git , GitHub
3	Read: Ch. 2	Read: Ch. 3, 4	Python : modules, types, logic
4	Read: Ch. 5	Read: Ch. 17	Python : functions, structure, debugging
5	Read: Ch. 6	Read: Ch. 18	Python : classes, testing
6	Read: Ch. 7		Python : visualization, Jupyter
7	Read: Ch. 9		Efficient python: arrays and numpy (Midterm project assigned)
8	<i>No Class</i>	<i>No Class</i>	Spring Break
9	Read: Ch. 10		Efficient python: managing data (HDF5)
10	Read: Ch. 11		Efficient python: data structures (Midterm project due)
11	Read: Ch. 12		Efficient python: parallelization
12	Numba Quickstart	Numba Videos	Efficient python: compiling with numba
13	Read: Ch. 20		Publication: \LaTeX and Jupyter
14			From scipy to MATLAB (Final project assigned)
15			MATLAB and Julia
16	<i>No Class</i>	Finals Week (Final project due)	