PHYS220/MATH220/CPSC220: SCIENTIFIC COMPUTING I

Spring 2018

Instructor: Dr. Justin Dressel

Email: Time: Tue 1:00 – 2:15pm

Place: 110 Hashinger Science Center

Office: 110 Hashinger Science Center

Office Hours: By appointment.

Course Page: https://github.com/chapman-phys220-2018s

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: None in favor of *free* web resources.

Python/SciPy Tutorial: http://www.scipy-lectures.org https://lectures.quantecon.org/py/learning_python.html

LATEXTutorial: https://www.latex-tutorial.com

bash Tutorial: http://linuxcommand.org/lc3_learning_the_shell.php

vim Tutorial: https://openvim.com

git Tutorial: https://tutorialzine.com/2016/06/learn-git-in-30-minutes

https://try.github.io

http://tom.preston-werner.com/2009/05/19/the-git-parable.html

MATLAB Tutorial: http://www.mathworks.com/help/matlab/getting-started-with-matlab.html

julia Tutorial: https://lectures.quantecon.org/jl/learning_julia.html
http://ucidatascienceinitiative.github.io/IntroToJulia/

sage Tutorial: https://doc.sagemath.org/html/en/tutorial/

Optional Textbooks:

Effective Computation in Physics, Scopatz & Huff, 2015.

https://physics.codes

Elegant SciPy: The Art of Scientific Python, Nunez-Iglesias et al., O'Reilly, 2017.

https://github.com/elegant-scipy/elegant-scipy

Hands-On Machine Learning with Scikit-Learn & TensorFlow, Géron, O'Reilly, 2017.

https://github.com/ageron/handson-ml

Grading Policy:

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

Organization:

This course involves building a set of professional skills, which means 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, which is documented according to industry standards, bug-free, unit-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 lecture time will be spent solving interesting physical problems, putting what you have read from the free web resources into practice. Similarly, homework will be a more challenging extension of what is covered in class for additional practice. The midterm and final projects will be more substantial, requiring a synthesis of all topics learned in the course.

GitHub:

Homework will be assigned and collected via git using http://www.github.com and Git Classroom. Your first task will be to ensure that you have an account, and know how to use it. The GitHub Organization for the course will be http://github.com/chapman-phys220-2018s.

Slack:

Group discussion and contact with the professor will be facilitated by Slack, at http://scststudents.slack.com. Your second task will be to ensure that you have an account. Please notify the instructor if you need to be invited. The channel for this course will be #phys220-18s and is set to auto-notify the instructor. Note that this is a public forum, but private chats are also available.

CoCalc (formerly SageMathCloud):

For ease of compatibility, we will be using http://cocalc.com as a browser-based development solution. Your third task is to ensure that you have an account, and that you inform the instructor of your username so that you may invited to the course project. Please use your Chapman email when registering your account, and choose a username such that your real name is clear. Your account will give you access to a virtual Linux machine running Ubuntu, complete with an accessible bash terminal, text editors like vim or nano or emacs, LaTeX, Jupyter notebooks, Numeric Python, Scientific Python, Pandas, C, C++, Julia, Octave, and many other useful tools: http://tutorial.cocalc.com/students/ You are welcome to use your own computer in addition to CoCalc, but it is your responsibility to install all software and ensure compatibility with CoCalc.

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 (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, students will:

- 1. Demonstrate knowledge and understanding of basic mathematics and physical principles used to model natural phenomena.
- 2. Demonstrate ability to convey physical concepts with mathematical expressions and/or computation, and effectively derive quantitative predictions from a model through mathematical/computational analysis.
- 3. Demonstrate competency in using computer tools.
- 4. Demonstrate the ability to apply advanced knowledge of advanced mechanics, electromagnetism, thermodynamics and quantum physics to the solution of problems in physics.
- 5. Demonstrate the ability to effectively communicate information, scientific or otherwise, in both written and verbal form.
- 6. Demonstrate the ability to write clear, organized and illustrated technical reports with proper references to previous work in the area.
- 7. Demonstrate the skills and motivation for continued self-education.

Chapman University Academic Integrity Policy:

Chapman University is a community of scholars which 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 not be tolerated anywhere in the university. At their discretion the faculty may submit work to plagiarism detection software, such as www.turnitin.com for review.

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 or http://www.chapman.edu/students/studenthealth-services/disability-services if you have questions regarding this procedure, or for information and 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 Chapmans Harassment and Discrimination Policy: http://ow.ly/XEwTu 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 here: http://www.chapman.edu/students/health-and-safety/psychological-counseling/

Approximate Course Outline:

| Week | Topics/Notes |
|------|--|
| 1 | CoCalc, bash, vim, git, GitHub |
| 2 | ipython, Jupyter notebooks, LATEX |
| 3 | Functions, modules, documentation, unit testing, Travis.ci |
| 4 | numpy arrays and pandas dataframes |
| 5 | Visualization with matplotlib and seaborn |
| 6 | Sequences, meshes, and finite difference equations |
| 7 | Interpolation and approximation (Midterm project assigned) |
| 8 | Spring Break |
| | |
| 9 | Symbolic computing with sympy (Midterm project due) |
| 10 | MATLAB vs. scipy |
| 11 | Monte Carlo techniques |
| 12 | Ordinary differential equations |
| 13 | Partial differential equations |
| 14 | numba, julia, and the LLVM (Final project assigned) |
| 15 | Work on final project — no class |
| 16 | Finals Week (Final project due) |