PHYS227 : Foundations of Scientific Computing

Spring 2016

Instructor:	Dr. Justin Dressel	**Time:**	Tue/Thur 10:00 – 11:15
Email:	dressel@chapman.edu	**Place:**	50 Hashinger Science Center

Office Hours: By appointment.

Course Page: `https://github.com/chapman-phys227-2016s`

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 and MATLAB are emphasized, along with brief introductions to Julia, Sage, and Mathematica.

Prerequisites: CPSC230, CPSC231

Main Reference: *A Primer on Scientific Programming with Python, 4th Edition*,
Hans Petter Langtangen, Springer, 2014.

Course Learning Outcomes:

1. Create professional reports in LaTeX, including proper section structuring, figures, and references. Augment these static reports with executable 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, emacs) 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.

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.

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, you are expected to keep up with the reading of the technical material *before* coming to class, so that you may arrive prepared to work. You are also expected to turn in professional quality work, which is documented, well-formatted, bug-tested, and well-written. Half of your job is solving interesting problems; the other half of your job is presenting the results of your work as a qualified professional.

The bulk of lecture time will be spent solving interesting physical problems together, putting what you have read 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.

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 `#phys227-sp16` and is set to auto-notify the instructor. Note that this is a public forum, but private chats are also available as required.

SageCloud:

For ease of compatibility, we will be using `http://cloud.sagemath.com` as a browser-based coding solution. Your third task is to ensure that you have an account, and that you create a project PHYS227 for this course. In addition to Sage, your account will give you access to a virtual Linux machine running Ubuntu, complete with an accessible bash terminal, `vim` and `emacs`, Jupyter notebooks, Numeric Python, Scientific Python, Pandas, C, C++, Julia, and many other useful tools.

Approximate Course Outline:

Week	Dates	Topics	Reading
1	2/2, 2/4	Git, Bash, SageCloud, Jupyter, LaTeX	§1.1—4.11 http://ow.ly/XETaR
2	2/9, 2/10	Arrays and visualization	§5.1—5.8
3	2/16, 2/18	Sequences and difference equations	§A.1—A.2
4	2/23, 2/25	Pandas and dataframes	§6.1—6.4 http://ow.ly/XFsdr http://ow.ly/XFs1H
5	3/1, 3/3	Discrete calculus	§B.1—B.4
6	3/8, 3/10	Introduction to differential equations	§C.1—C.5
7	3/15, 3/17	MATLAB vs. Scientific Python I (Midterm project assigned) *(Instructor at APS March Meeting)*	http://ow.ly/XFvld
8	3/22, 3/24	**Spring Break**	
9	3/29, 3/31	Introduction to classes	§7.1—7.7
10	4/5, 4/7	Monte Carlo techniques	§8.1—8.5
11	4/12, 4/14	Object-oriented techniques	§9.1—9.3
12	4/19, 4/21	Differential equations example	§D.1—D.3
13	4/26, 4/28	Differential equations continued	§E.1—E.3
14	5/3, 5/5	MATLAB vs. Scientific Python II (Final project assigned)	http://ow.ly/XFxWc
15	5/10, 5/12	Julia vs. Scientific Python	http://ow.ly/XFxBH

Chapman University Academic Integrity:

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.

Students with Disabilities:

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.

Equity and Diversity:

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.