PHY494: Computational Methods in Physics (Spring 2017)

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Course page:	see Blackboard
Web page:	http://becksteinlab.physics.asu.edu/learning/76/phy494-computational-physics

Contents

1 Course description

The course provides a practical introduction to using the computer as a tool to solve problems in physics. Students will learn how to work in a scientific computing environment (including software engineering "best practices"), to analyze a physical problem, select appropriate numerical algorithms to solve the problem, and to implement them. The course will introduce the students to computer graphics and object oriented design. Students will work in teams, critically evaluate their approaches and results, and present them in a professional manner to their peers. The instructor will introduce problems and guide students to their solution.

This is a three-credit hour course. It will be taught in a computer laboratory setting. The emphasis is on practical work, with the instructor initially introducing the problem, and the students then pursuing pre-structured programming exercises and projects. Assessment will primarily focus on projects, including group projects, in which students solve a problem as a small team and present their work as a short report and talk.

PHY 252 is a co-requisite

1.1 Content

The course does not require any previous programming experience. We plan to cover the following topics but depending on the class and special interest, this may change.

Working in a scientific computing environment

- Unix shell
- version control with *git*
- programming in *Python*; use of numerical libraries; publication-quality plotting
- if time permits: remote access and high performance computing (HPC) environments; queuing systems; parallel computing

Fundamentals of numerical approaches

- number representations and errors
- random numbers and Monte Carlo
- derivatives and integration
- linear algebra (matrix calculations, eigen problems)
- root-finding, minimization, data fitting
- solving ordinary differential equations (ODEs)
- partial differential equations (PDEs)
- Fourier analysis

Applications to physical problems

(Not all topics will be included in the class but can be introduced through projects.)

- chaotic pendulum, non-linear dynamics
- molecular dynamics
- Ising model
- electrostatics (Laplace and Poisson equation)
- heat and wave equations
- quantum mechanics (Schrödinger equation)
- fluid dynamics

1.2 Learning outcomes

Students will learn to program computers in order to solve physical problems. In particular, they will be able to write object oriented code in the open source Python programming language, which is widely used in science and engineering and in some of the biggest tech companies.

Students will also learn how to solve problems in teams and to communicate their work clearly and effectively.

By the completion of the course, students should be able to quickly apply their knowledge to problems they encounter in other courses and experimental and theoretical research projects.

1.3 Reading materials

The following texts are used:

1. Jay Wang, *Computational Modeling and Visualization of Physical Systems with Python* (2016). Wiley-VCH
2. Rubin H. Landau, Manuel J. Páez and Cristian C, Bordeianu. *Computational Physics—Problem Solving with Python* 3rd ed (2015). Wiley-VCH

Other online reading material and resources will be introduced during the course.

1.4 Grading and assignments

The course grade will be determined from individual and group work; instead of written exams, project work will be assessed.

20%	home work assignments (see 1.4.2)
40%	projects (see 1.4.3)
30%	final project (see 1.4.4)
10%	participation (see 1.4.5)

1.4.1 Grading policy

The full grade scale[1] from A+ down to E is used for the final course letter grade. Conversion from percentages (rounded to whole percentages) to a course letter grade will be carried out on a fixed scale at the end of the semester. The following letter grade conversions are guaranteed

[1] See `https://students.asu.edu/grades` for the meaning of the grades.

and you will always get at least the letter grade from the table below if your overall course percentage is sufficient:[2]

min	max	letter
97%	100%	A+
94%	96%	A
90%	95%	A−
87%	89%	B+
84%	86%	B
80%	83%	B−
76%	79%	C+
70%	75%	C
60%	69%	D
0%	59%	E

Please note:

- No credit will be given for late or unexcused homework.
- No credit will be given for just running provided code. Your are expected to modify, extend, and rewrite code.
- In case of documented medical or family emergencies you may be allowed to submit home work for credit after the due date. Contact the instructor within 48 hours after the due date of the home work to apply for an extension and provide documentation for the emergency.
- You may discuss home work problems with your peers but you must write and submit *your own work* (unless specifically instructed otherwise, e.g. for *group projects*).
  Always cite sources of material that is not your own, such as input from other students or code found on the internet or in books. (As an exception, you do not have to explicitly cite materials provided in the class.)
- When you submit work for yourself or as part of a group you do this with the understanding that the instructor can always elect to have you explain code and results and, depending on your explanation, adjust your grade accordingly.
- You submit home work reports electronically (PDF format) through BlackBoard. If you scanned your report make sure that its is legible; reports that are difficult to read might be returned un-graded with 0 points.
  Code and output (which are typically part of a home work assignment) should be submitted by the deadline to your GitHub code repository, using file locations and naming as instructed in the class.

1.4.2 Home work assignments

Typically, there will be one home work assignment per week. Home work will be due one week after it has been assigned, as specified on the assignment. It will be graded and returned. The

[2] It is, however, possible that the grading schema will be adjusted at the end of the semester to reflect overall class performance and other circumstances. Any of these adjustments will not reduce your grade guaranteed by the table above, i.e. your grade would either remain the same or improve due to these adjustments.

lowest scoring homework grade will be dropped from the grade calculation. The home work is an integral part of the course.

Home work assignments may also consist of a small project that involves programming, producing output and handing in a short report. The report should contain the equations that are solved, the computational method, the results (in form of graphs and/or tables), and a critical discussion. Code and output should be submitted to your GitHub code repository.

1.4.3 Group projects

Students will complete 2 to 3 projects. The projects may be carried out individually or in teams, depending on the problem setting. In group projects, students have to solve a physics problem together, submit code and output for the group, and individually hand in a written report in the style of a "letter" paper. Individual projects are similar to extended "project homeworks".

1.4.4 Final project

Students will undertake final projects as an extended application of the topics learned in the class. Final projects will be carried out in teams. Results will be presented as a poster in a final poster session together. Students will be assessed based on the code and output in the GitHub repository and their individual presentations at the poster.

1.4.5 Participation

Students may also be engaged in other activities such as peer instruction and peer grading. Participation in these activities and in class will contribute to the total course grade.

2 Conduct

2.1 Attendance and class disruption

Students are expected to attend every scheduled class period and to be punctual. You are responsible for all material covered in class, even in your absence! If you are absent, obtain class notes and handouts from your fellow students.

Use of cell phones, beepers, smart phones, tablets, and other electronic devices *is prohibited in class* unless used for participation in exercises or taking lecture notes. Devices must be silenced before entering.

2.2 Lectures and lecture material

Lecture materials will be made available under a Creative Commons CC-BY licence, which allows distribution with attribution. Some materials from third parties might come under different licenses that do not allow public posting or dissemination.

Recording of lectures or taking pictures during lectures is prohibited unless explicit and specific written permission has been granted by the instructor.

2.3 Blackboard

Each student has access to the *PHY 494* course page. You are expected to check this site on a daily or near-daily basis. Important announcements, course documents (syllabus and

general information), presentations and other course materials will be posted here throughout the semester. You will also find **home work assignments** here.

2.4 Communication

You can see your instructor during office hours or send an e-mail[3]. E-mails will generally be answered within two business days. Although effort will be made to also respond sooner to urgent e-mails, no guarantee can be given that e-mails will be answered in time e.g. on the night before a home work due date—make sure that you ask well in advance of any critical dates.

2.5 Academic dishonesty

Academic honesty is expected of all students in all examinations, papers, laboratory work, academic transactions and records. The possible sanctions include, but are not limited to, appropriate grade penalties, course failure (indicated on the transcript as a grade of E), course failure due to academic dishonesty (indicated on the transcript as a grade of XE), loss of registration privileges, disqualification and dismissal. For more information, see http://provost.asu.edu/academicintegrity.[4]

Academic dishonesty will not be tolerated in this course. There are severe sanctions for cheating, plagiarizing and any other form of dishonesty, including a permanent XE in the student record. In the *Student Academic Integrity Policy manual*, ASU defines "*plagiarism* [as] using another's words, ideas, materials or work without properly acknowledging and documenting the source. **Students are responsible for knowing the rules governing the use of another's work or materials and for acknowledging and documenting the source appropriately.**" In particular, plagiarizing code or results of other students is a severe offence that will be sanctioned.

All students are expected to visit http://graduate.asu.edu/beintheknow in order to educate themselves on academic integrity.

3 Withdrawal policy

The withdrawal policy is established by the university.

4 Disability policy

Disability Accommodations Qualified students with disabilities who will require disability accommodations in this class are encouraged to make their requests to the instructor at the beginning of the semester either during office hours or by appointment. **Note:** Prior to receiving disability accommodations, verification of eligibility from the Disability Resource Center (DRC) is required. Disability information is confidential.

Establishing Eligibility for Disability Accommodations Students who feel they will need disability accommodations in this class but have not registered with the Disability Resource

[3] E-mails are expected to be written in a professional tone. See *Scientific Communication: E-mail* at http://www.nature.com/scitable/topicpage/e-mail-13953985 for what this means. Start your subject with "*PHY494: ...*".

[4] This paragraph is required by ASU and outlines the *minimum* university-wide policy.

Center (DRC) should contact DRC immediately. Their office is located on the first floor of the Matthews Center Building. DRC staff can also be reached at: 480-965-1234 (V), 480-965-9000 (TTY). For additional information, visit http://www.asu.edu/studentaffairs/ed/drc. Their hours are 8:00am to 5:00pm, Monday through Friday.

A History of changes to this document

Amendments to the original initial version of this Syllabus are recorded here. See also the date at the top of this document.

January 10, 2016 initial version