PHY432: Computational Methods in Physics (Spring 2022)

Oliver Beckstein

January 10, 2022

Instructor:	Dr Oliver Beckstein
Lecture:	Tue/Thu 1:30pm–2:45 pm
Classroom:	PSH 355
Phone:	(480) 727-9765
E-mail:	oliver.beckstein@asu.edu (subject: *PHY 432...*)
Instructor Office hours:	Thu 10:00 am–11:00 am (Zoom)
Instructor Office:	PSF 348
TA:	Chenou Zhang, czhan178@asu.edu (Zoom)
TA Office hours:	Wed 2:00 – 3:00 pm
Course page:	see Canvas
Web page:	`https://becksteinlab.physics.asu.edu/learning/146/phy432-computational-physics`

In order to schedule an appointment outside of the posted office hours, email the instructor at least two days in advance.

Contents

1. Course description and overall objectives

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.

Programming experience equivalent to PHY 202 is required.

1.1. Content

The course requires programming experience in the Python programming language (at the level of an introductory class such as PHY 202). Students will learn to use the Python programming language, which is widely used in science and engineering and in some of the biggest tech companies, to solve problems in Physics. They will also be introduced widely used software engineering best practices and tools such as using the command line, version control, and testing.

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

Fundamentals of numerical approaches

- number representations and errors
- 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
- random numbers and Monte Carlo

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

1. Students will learn to program computers in order to solve physical problems. In particular, they will be able to read and write code in the

Python programming language.

2. They will be able to use the git version control system to manage code and to use a remote git repository.

3. They will be able to use the Unix shell to navigate the file system and perform simple file and directory manipulations from the command line.

4. They will be able to use a text editor to write code.

5. They will have a basic understanding of the benefit of testing code with unit tests and be able to run such tests when provided.

6. They will be able to use functionality in common scientific Python libraries such as `math`, `numpy`, `matplotlib`, and `scipy`.

7. They will be able to implement a given numerical algorithm in Python and run it.

8. 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 apply their knowledge to problems they encounter in other classes and experimental and theoretical research projects.

1.3. Reading materials

The class broadly follows the book

1. Jay Wang, *Computational Modeling and Visualization of Physical Systems with Python* (2016). Wiley-VCH

It is recommended for additional in-depth studying but students are not required to purchase the book.
The following texts are also useful but are not required:

resume Anthony Scopatz and Kathryn D. Huff, *Effective Computation in Physics. Field Guide to Research with Python.* (2015) O'Reilly

resume 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.

30%	home work assignments (see 1.4.2)
30%	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 and you will always get at least the letter grade from the table below if your overall course percentage is sufficient:[2]

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

[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.

min	max	letter
97%	100%	A+
94%	96%	A
90%	93%	A−
87%	89%	B+
84%	86%	B
80%	83%	B−
76%	79%	C+
70%	75%	C
60%	69%	D
0%	59%	E

Grades will be posted to Canvas and feedback will be provided either through Canvas or as files in your assignment GitHub repository (see Section 2.2).

Please note:

- No credit will be given for late or unexcused homework.
- No credit will be given for just running provided code. You 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.
- *This class will require you to create an account on GitHub* `https://github.com` because we will continually make use of the site for

cloud-based git repositories. You will have a private repository for your home work assignments for the duration of the class (see Section 2.2 for more details).

- You submit home work reports electronically as instructed in the assignment. This can mean through Canvas or in your GitHub repository as, for instance, a PDF or text file.
  Code and output (which are typically part of a home work assignment) should be submitted by the deadline to your GitHub code repository (at `https://github.com/ASU-CompMethodsPhysics-PHY432`), using file locations and naming as instructed in the class and in the assignment.
- 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.

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 lowest scoring homework grade will be dropped from the grade calculation. The home work is an integral part of the course. Home work assignments will be initially posted on Canvas (Section 3.3) and then in a git repository hosted on GitHub (see Section 2.2); students will be taught how to access the git repositories.

Home work assignments typically require writing of programs, running the written code, and analysing the output. 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.

Some assignments will contain tests that can and should be run by the student to check their solution. Passing tests are a good sign that the solution is complete but no guarantee that the solution will be graded with full points. Final grading decisions are at the discretion of the grader and instructor.

At the discretion of the instructor, Makeup Assignments may be provided. Students will be able to hand in a Makeup Assignments to be graded. Makeup Assignments are optional and students are never required to hand one in. The grade of a Makeup Assignment will replace the lowest other homework assignment grade if doing so improves the student's grade. No extensions will be granted for submission deadlines of Makeup Assignments.

1.4.3. Midterm projects

Students will complete two midterm projects. The projects may be carried out individually or in teams, depending on the problem setting. *Midterm Project 1* is carried out by each student individually. *Midterm Project 2* is a team project. For Midterm projects, students must solve a physics problem, submit working code, and produce a written report in the style of a "letter" paper.

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 pre-recorded presentation with participation of all team members. Students will be assessed based on the code and output in the GitHub repository, their presentations, and any other written materials as detailed in the Final Project handout.

1.4.5. Participation

Students may also be engaged in other activities such as solving problems during class time. Participation in these activities and in class will contribute to the total course grade.

It is expected that all students attend class. The instructor may decide to take attendance and factor attendance into the participation grade whereby 50% of the participation grade will be awarded based on attendance in a manner proportional to attended classes.

1.5. Weekly lesson plan

Week	Unit	Lesson	Assignment
1	0	Installing the environment	
	1	The Unix Shell	HW 1
2	2	Git basics	
	3	Programming in Python refresher	HW 2
3	3	Python: Modularization	
	4	Debugging primer	HW 3
4	4	NumPy and matplotlib	
	4	Stochastic dynamics with NumPy	HW 4
5	5	Number representations and errors	
	6	Differentiation	HW 5
			Midterm Project 1
6	7	Ordinary Differential Equations (ODEs)	HW 6
7	8	ODE Applications: Celestial mechanics and Molecular Dynamics	HW7
8	8	ODE Applications: Baseball physics	HW 8
			Midterm Project 2
9	9	Root finding by trial-and-error	HW 9
10	10	Linear Algebra	HW 10
11	11	Partial Differential Equations (PDEs)	HW 11
12		*Final Project Pitches*	*Final Project*
	12	Solving PDEs with time stepping	HW 12
13	12	Advanced PDE time stepping algorithms	
	13	PDEs: Wave equation	HW 13
14	14	Special Topic: SVD and curve fitting	
	15	Special Topic: FFT and signal processing	
15	16	Monte Carlo simulations	
	16	MC application: 2D Ising model	
16		*Final Project Presentations*	*Final Project*

2. Technology support

2.1. Laptop

For the class you **must have a computer** to follow programming exercises and homework and project assignments. During each class you will need your laptop as the class is taught in a studio setting.

Own laptop Ideally, you bring your own laptop. During the first lesson we will walk you through the installation instructions. The instructor and TA will be available to help with trouble shooting. We also maintain a FAQ for installation questions at `https://github.com/ASU-CompMethodsPhysics-PHY494/PHY494-resources/wiki`.

ASU machines If you can't use your own machine:

1. We provide you with a working laptop during class.
2. For assignments you should use the public iMac computers in the Tempe Computing Commons 102 (CPCOM 102). Follow the instructions on using CPCOM 102.

2.2. GitHub

This class will require you to create an account on GitHub `https://github.com` because we will continually make use of the site for cloud-based git repositories. You will have a private repository for your home work assignments for the duration of the class. You will be able to copy all content from this repository if you wish to have it after the class when your private repository will be deleted again. Your repository will be available under `https://github.com/py4phy`. A private repository is only visible to the student and the instructors. All communication with GitHub is encrypted via SSL; students are responsible for guarding their own GitHub account. Enabling two-factor authentication (2FA) is recommended.

Group projects will also use private repositories for groups of students. The Final Project will use a public repository in order to introduce students to programming in an open source context and provide an opportunity to show-case their work; however, students may request a private repository for the Final Project.

2.3. Class web pages

Almost all content for the class will be made available through the `https://py4phy.github.io/PHY432/` web pages. A modern web browser is required to access these pages. The pages will be build incrementally as the class progresses. Content will be archived and will remain accessible after the conclusion of the class under a different URL.

3. Conduct

3.1. 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.

3.2. 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. See Recording for notes on how recordings will be made available.

3.3. Canvas

Each student has access to the *PHY 432* course pages on Canvas. 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, although you will have to follow the specific instructions of the assignments on how to obtain, e.g., starter code from the course GitHub repository.

Recordings of the class meetings will also be available on Canvas as described under Recording.

3.4. Copyrighted materials

Students must refrain from uploading to any course shell, discussion board, or website used by the course instructor or other course forum, material that is not the student's original work, unless the students first comply with all applicable copyright laws; faculty members reserve the right to delete materials on the grounds of suspected copyright infringement.

3.5. 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.

[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 "*PHY432:* ...".

3.6. Absences and late submissions

Attendance and participation in class activities is an essential part of the learning process, and students are expected to attend class regularly. All students will be given ample notice for deadlines for home work assignments and projects and it is expected that students coordinate their other activities with their class obligations in such a way that they will be able to hand in assignments and project before or by the given deadlines. In general, late submissions will be graded with 0 points.

Some absences are, however, unavoidable. Excused absences for classes will be given without penalty to the grade in the case of **(1) a university-sanctioned event** [ACD 304-02]; **(2) religious holidays** [ACD 304-04; a list can be found here `https://eoss.asu.edu/cora/holidays`]; (3) **work performed in the line-of-duty** according to [SSM 201-18]; and **(4) illness, quarantine or self-isolation related to illness** as documented by a health professional; (5) **other family or medical emergencies**.

Anticipated absences for university-sanctioned events, religious holidays, or line-of-duty activity should be communicated to the instructor by e-mail at least 7 days before the expected absence.

Absences for illness, quarantine or self-isolation related to illness should be documented by a health professional and communicated to the instructor as soon as possible by e-mail.

For any other emergencies students should contact the instructor by email as soon as possible and ideally *before* any deadline to secure an extension. Written documentation for emergencies (such as a doctor's note) will be required on a case-by-case basis.

If there is a disagreement as to whether an absence should be accommodated, you may contact the academic unit chair immediately for resolution.

Excused absences do not relieve students from responsibility for any part of the course work required during the period of absence. The instructor will provide accommodations that may include participation in classes remotely, access to recordings of class activities, and make-up work (see also Section Accommodations).

3.7. Accommodations

Please note that this class is listed as an in-person (immersion) class. A streaming option is provided *as an accommodation* for necessary absences. If you feel you are vulnerable to COVID-19 please contact Student Accessibility and Inclusive Learning Services (SAILS) to discuss possible accommodations such as following the class remotely.

3.7.1. Streaming

In case you cannot attend class in person as a result of illness or possible exposure to infectious disease, you may participate in this class remotely via Zoom stream. To participate remotely, use the class Zoom link available in Canvas. You must be *authenticated with your asu.edu account in Zoom* in order to stream the class.

If you use the streaming option **you are still required to inform the instructor of your absence** as defined in Absences and late submissions.

All students should bring a mobile device to class regularly to allow participation with colleagues via Zoom as necessary.

3.7.2. Recording

Note that class sessions will be recorded and recordings provided to enrolled students, instructors or instructional support personnel. If you have concerns about being recorded, please contact the course instructor.

Recordings of all class sessions will be posted in Canvas for *all students* to access for reviewing course materials.

3.8. Academic integrity

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 https://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 https://graduate.asu.edu/current-students/policies-forms-and-deadlines/academic-integrity in order to educate themselves on academic integrity.

3.9. Face coverings

The ASU Face Cover Policy currently requires the wearing of face covers in the classrooms, teaching laboratories, studios and workshop settings. **The space for this class has been designated as a space requiring face covers.** Please wear a face covering (such as N95 mask, KN95 mask, medical-grade mask) over your nose and mouth at all times during class for the health and safety of yourself and others.

4. Withdrawal policy

The withdrawal policy is established by the university.

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

5. 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 Student Accessibility and Inclusive Learning Services (SAILS) is required. Disability information is confidential.

Establishing Eligibility for Disability Accommodations All students requesting accommodations must work with the Student Accessibility and Inclusive Learning Services (SAILS), the central location for establishing eligibility and obtaining services and accommodations for qualified students with disabilities. You may contact SAILS at 480-965-1234 or via email at Student.Accessibility@asu.edu. For additional information, visit `https://eoss.asu.edu/accessibility`.

6. Policy against threatening behavior

This class adheres to ASU's policy against threatening behavior (Student Services Manual SSM 104-02 "Handling Disruptive, Threatening or Violent Individuals on Campus"):

All incidents and allegations of violent or threatening conduct by an ASU student (whether on-or off campus) must be reported to the ASU Police Department (ASU PD) and the Office of the Dean of Students. If either office determines that the behavior poses or has posed a serious threat to personal safety or to the welfare of the campus, the student will not be permitted to return to campus or reside in any ASU residence hall until an appropriate threat assessment has been completed and, if necessary, conditions for return are imposed. ASU PD, the Office of the Dean of Students, and other appropriate offices will coordinate the assessment in light of the relevant circumstances.

7. Title IX: Sexual discrimination and harassment

Title IX is a federal law that provides that no person be excluded on the basis of sex from participation in, be denied benefits of, or be subjected to discrimination under any education program or activity. Both Title IX and university policy make clear that sexual violence and harassment based on sex is prohibited. An individual who believes they have been subjected to sexual violence or harassed on the basis of sex can seek support, including counseling and academic support, from the university. If you or someone you know has been harassed on the basis of sex or sexually assaulted, you can find information and resources at https://sexualviolenceprevention.asu.edu/faqs.

As a mandated reporter, I am obligated to report any information I become aware of regarding alleged acts of sexual discrimination, including sexual violence and dating violence. ASU Counseling Services, https://eoss.asu.edu/counseling, is available if you wish discuss any concerns confidentially and privately.

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 7, 2022 initial version

January 10, 2022 updated lesson plan