PHYS-4007/5007: Computational Physics
Syllabus — Spring 2023

Lecturer (E-mail):	Dr. Donald Luttermoser (lutter@etsu.edu)
Office (Phone):	280 Brown Hall (439-7064)
Course ID:	PHYS-4007 (undergrad-level), PHYS-5007 (grad-level)
Credit Hours:	4
Prerequisites:	PHYS-2110/20 or MATH-2120
Lecture Locations:	Brown Hall 264 (T) & Brown Hall 266 (WF)
Lecture Times:	T 11:45 a.m. – 1:05 p.m.
	W F 3:10 p.m. – 4:05 p.m.
Office Hours:	By Appointment
Course Web Page:	https://faculty.etsu.edu/lutter/courses/phys4007/
Textbooks:	(1) *Computational Physics: Problem Solving with Python, 3rd Edition* (2015) Landau, Páez, & Bordeianu
	(2) *Learning Scientific Programming with Python, 2nd Edition* (2015) Christian Hill

Course Outline

Week	Topics	Textbook Readings*
Jan 16	I. An Intro to Scientific Computing (**No class on 1/16,17**)	Chaps 1, 2
Jan 23	II. Choosing a Programming Language	Class Notes
Jan 30	III. Preparing Scientific Manuscripts (**No class on 2/1**)	Class Notes
Feb 6	IV. Error Analysis and Uncertainties (**No class on 2/8**)	Chap 3
Feb 13	V. Methods of Data Fitting	Chap 7
Feb 20	Methods of Data Fitting (cont.)	Chap 7
Feb 27	VI. Numerical Differentiation and Integration	Chap 5
Mar 6	Integration (cont.)	Chap 5
Mar 10	**Take-Home Midterm Exam Due**	
Mar 13	**No classes – Spring Break**	
Mar 20	VII. Matrices and Solutions to Linear Equations	Chap 6
Mar 27	Matrices (cont.)	Chap 6
Apr 3	VIII. Numerical Solution of ODEs (**No class on 4/7**)	Chap 8
Apr 10	IX. Computing Trajectories	Chap 9
Apr 17	X. Computing Orbits	Class Notes
Apr 24	**Class Project Due** (Optional for Extra Credit)	
Apr 24	XI. Numerical Solution to PDEs	Chap 19
May 4	**Take-Home Final due by 5 p.m.**	

* Landau, Páez, & Bordeianu Textbook

Course Description

Computational Physics (PHYS-4007 for undergraduate credit, PHYS-5007 for graduate credit) is designed to cover techniques used in modeling physical systems numerically and analyzing data. It is designed to help the students gain experience with **programming languages** in carrying out this work. It is also important to know how these programming languages are accessed in an **operating system**. **Note however that this is not a course in computer programming!** Instead, this course is designed to use computer programming to solve scientific problems in physics and astronomy. Two of the most common programming languages used in these sciences are FORTRAN and Python. In addition, many astronomers and astrophysicists use the Interactive Data Language (IDL) in their research. Techniques will be developed to numerically differentiate and integrate, and to solve systems of linear equations, ordinary differential equations (ODE), trajectory and orbit problems with numerical methods, and finally partial differential equations (PDE). The students also will be introduced to data fitting techniques. Note that the theoretical foundations to each of these subjects will be introduced to the students prior to focusing on the numerical techniques.

Students should have already taken PHYS-2110/20 (*Technical Physics I & II*) and/or MATH-2120 (*Differential Equations*) before taking this course. Though previous computer programming experience is not required, such experience will be beneficial to the student. We will primarily be using the Python programming language throughout most of the course, though we will occasionally also use FORTRAN since it is widely used in physics and astronomical research. Tutorials on the use of FORTRAN, Python, and IDL are given in **Appendices B, C**, and **D**, respectively, of the course notes. **Appendix E** contains a reference guide to the C programming language for those of you interested in using this language.

Computational Physics is a problem-solving course, that is, the measure of a student's progress is demonstrated by the ability to solve numerical problems in physics and astronomy using computer programming methods. Upon completion of this course, the student will possess the basic knowledge of numerical modeling and data analysis that may be required for graduate school or in a position at a technical corporation.

In this course, the student will primarily be using the Linux operating system on the computers in Brown Hall Room 264. Besides learning how to solve numerical problems with a computer, the student also will gain experience writing manuscripts in a scientific journal style using the mark-up language LaTeX. As a matter of fact, this syllabus and all of the course notes are written in LaTeX with the graphics being created in IDL. LaTeX is used by a large number of professional journals, conference proceedings, and textbooks in both the physical sciences and mathematics. Each student will be given a sample LaTeX file to help them get started using this beautiful mark-up language.

Two textbooks are required for the course: (1) *Computational Physics, Problem Solving with Python, 3rd Edition* by Rubin H. Landau, Manuel J. Páez and Cristian C. Bordeianu, published in 2015 by John Wiley, and Sons, Inc.; and (2) *Learning Scientific Programming with Python, 2nd Edition* by Christian Hill published in 2015 by Cambridge University Press. Although not required, students may wish to purchase the book: *Guide to LaTeX, 4th Edition* by Helmut Kopka and Patrick W. Daly, published in 2003 by Addison-Wesley Publishing Company. Besides this book, it also might be a good idea to buy a book dealing with one of the programming languages that are used in physics and astronomy. For Python, I recommend Introducing Python: Modern Computing in Simple Packages by Bill Lubanovic published in 2015 by O'Reilly. Below is a list of good reference books in Computational Physics and Programming Languages. Most of these can be found on Amazon (http://www.amazon.com/).

- *Computational Physics*, N.J. Giordano, 1997, Prentice-Hall.
- *Physics by Computer*, W. Kinzel & G. Reents, 1998, Springer-Verlag.
- *Fortran 90 for Engineers & Scientists*, L.R. Nyhoff & S.C. Leestma, 1997, Prentice-Hall.
- *Problem Solving and Structured Programming in Fortran 77*, E.B. Koffman & F.L. Friedman, 1990, Addison-Wesley.
- *Introducing Python: Modern Computing in Simple Packages*, B. Lubanovic, 2015, O'Reilly Media, Inc.
- *Python for Data Analysis*, Wes McKinney, 2013, O'Reilly Media, Inc.
- *Python and matplotlib essentials for scientists and engineers*, Matt A. Wood, 2015, Morgan & Claypool Publishers.
- *Practical IDL Programming*, L.E. Gumley, 2002, Morgan-Kaufmann.
- *A Book on C, 3rd Edition*, A. Kelley & I. Pohl, 1995, Benjamin Cummings Publishing.
- *Introducing C++ for Scientists, Engineers and Mathematicians*, D.M. Capper, 1994, Springer-Verlag.
- *Unix for Programmers and Users*, G. Glass, 1993, Prentice-Hall.
- *The Official ubuntu Book, 8th Ed.*, M. Helmke & E.K. Joseph, 2015, Prentice-Hall.

In the world of business, *object-oriented programming*, primarily using the C++ programming language, is often used. However, in the scientific world (and in high-tech industries), what some scientists referred to as *structured programming* (mainly FORTRAN and some C) is typically used. In both the astronomical and medical fields, the Interactive Data Language (IDL) is widely used, mainly due to its rich graphics capabilities. In recent times, the popularity of Python has risen in physics and astronomy. Note that there are many large codes in the scientific community, most of them written in FORTRAN 77 due to its number-crunching capabilities, that are likely to stay in use for a long period of time. That is the main reason for covering a bit of FORTRAN 77 in this course as we learn computational physics. Many of the PCs in Brown Hall 264 will have LaTeX, FORTRAN 77 (the GNU gfortran compiler), and Python on the 'Linux side' of these machines.

Computer modeling is very complicated and requires years of training to become proficient at it using just one computer language. I have decades of experience using both FORTRAN and IDL programming languages to carry out my research. I want each student to learn how to program to solve problems numerically using computer programs they have written or modified themselves. This type of work can be very frustrating, but becomes very stimulating when one succeeds at it.

On Campus Attendance is Required this Semester

Unlike the recent COVID-19 Pandemic years, you will be required to attend class on campus in Brown Hall 370. **The exception to this is if you have been tested positive with COVID-19,** or you are sick from some other infection. Then you can watch the lecture via Zoom. You will not be required to wear masks in the classroom, however, **I will require mask wearing if you get within 5 feet of me.**

Please note your professor is *immune-compromised* due to the medications he is taking.

For providing information to keep the ETSU community safe and communicating updates regarding policy changes, please visit the Bucks are Back web site:

https://www.etsu.edu/coronavirus/

It remains the best place to find updated information regarding ETSU's protocols and safety measures during the pandemic.

D2L Course Website

I typically do not use D2L in this course, however, there may be a few occasions where I will need to post something for the class. If that's the case, a link to the ETSU D2L Login web page is included on the course web page at

https://faculty.etsu.edu/lutter/courses/phys4007/index.htm.

Homework, Exams, and Computer Project

The students will be graded on their performance on a **Midterm** and a **Final** — the Final is not comprehensive. Both of these tests will be take-home and passed out a week prior to their due date. Four to six **homework sets** will be assigned throughout the semester. In addition, students taking the 001 section of this course have the option of carrying out a course computer project. Undergraduates taking the honors section (088) and graduate students taking the graduate course (PHYS-5007) **are required to do this project.** The **Computer Project** will require a term paper to be submitted by the due date describing the code and results. Undergraduate students taking the 001 section can earn up to 20% additional extra-credit points by completing this project. The formulas in the **Grading Policy** section at the end of this syllabus give the various percentages of the homework, midterm, final, and computer project used to determine your course grade.

The students will be instructed in the use of the mark-up language LaTeX which is used in many physical science and mathematical journals. The students will be required to write their optional term paper with LaTeX. A single-sided, 8 to 12 page term paper will be required for this computer project. I will supply a list of possible projects in case you have trouble coming up with a project on your own. Exams, homework assignments, the project paper and associated codes **must** be turned in on the due date no later than 5 p.m. on those days. **There are no exceptions to that rule!** Anything turned in within three days after the due date (again by 5 p.m.) will be reduced by one full grade for that assignment, exam, or project. Anytime after that three day period will result in a zero for that late item.

Grading Policy

The grading system will be based by the following criteria for **non-honors undergraduate students**:

Course Grade = 40%*(Homework) + 30% *(Midterm) + 30% *(Final)

The grading system will be based by the following criteria for **honors undergraduate and graduate students**:

Course Grade = 30%*(Homework) + 25% *(Midterm) + 25% *(Final)
+ 20%*(Class Project)

Each of the items in the formulae above represent the normalized score for the given item. The final grades will be based on the following scales:

The **Undergraduate Student Scale**:

			A	=	90% or better	**A−**	=	88–89.9%
B+	=	86–87.9%	**B**	=	76–85.9%	**B−**	=	73–75.9%
C+	=	70–72.9%	**C**	=	62–69.9%	**C−**	=	59–61.9%
D+	=	56–58.9%	**D**	=	50–55.9%			
			F	=	Less than 50%			

The **Honors Undergraduate and Graduate Student Scale**:

			A	=	90% or better	**A−**	=	88–89.9%
B+	=	86–87.9%	**B**	=	76–85.9%	**B−**	=	73–75.9%
C+	=	70–72.9%	**C**	=	62–69.9%	**F**	=	Less than 62%

Note that a failing grade also will be given if the student has engaged in any form of academic dishonesty.

Mental Health: Students often have questions about mental health resources, whether for themselves or a friend or family member. There are many resources available on the ETSU Campus, including: ETSU Counseling Center (423) 439-4841; ETSU Behavioral Health & Wellness Clinic (423) 439-7777; ETSU Community Counseling Clinic: (423) 439-4187.

- If you or a friend are in immediate crisis, call 911.
- Available 24 hours per day is the National Suicide Prevention Lifeline: 1-800-273-TALK (8255).