PHYSIC 362 Computational Science **Spring 2021**

Instructor:	Olga Goulko	Lectures:	Tu&Th 2-3:15pm Eastern
Office hours:	Tu&Th 4:30-6pm	Lab:	Fri 2-4pm Eastern
Email:	`olga.goulko@umb.edu`	Homework due:	Fri 2pm Eastern

This course provides an introduction to the uses of computational tools in physics and other natural sciences. While we study numerical methods and programming, the emphasis is on computation as an aid to understanding physical systems. Pre-reqs: PHYSIC 113, Math 140, CS 110 or permission of the instructor. This course is combined with PHYSIC 697. Credits: 4

Expected student learning outcomes

- being able to turn mathematical equations into code
- being able to make use of standard algorithms for numerical modeling of physical systems
- being able to create simulations of physical systems
- being able to use computational methods to read, write and manipulate data
- becoming familiar with the Python programming language and useful programming tools
- acquiring good programming style for scientific problems
- being able to create useful and informative scientific plots

These skills are essential for all areas of physics and will be very useful for your future studies, as well as academic and professional careers.

Course topics

The topics and timing may change as the semester develops. The mid-term exam is tentatively scheduled during lecture 14.

1. Scientific computing basics (Week 1-3)
    - Role of computational physics (Lecture 1)
    - Good programming practices (Lecture 2)
    - Review of Python basics (Lecture 3-4)
    - Algorithms, computational efficiency, numerical errors and accuracy (Lecture 5)
2. Numerical methods (Week 3-11)
    - Linear algebra: matrix operations, linear equations, eigenvalue problems (Lecture 6-8)
    - Non-linear equations, root finding, function optimization (Lecture 9-10)
    - Data fitting: interpolation and extrapolation, splines, least-squares (Lecture 11-16)
    - Numerical integration (Lecture 17-18)
    - Ordinary differential equations: Euler, midpoint, Runge-Kutta (Lecture 19-20)
    - (Fast) Fourier transform (Lecture 21-22)
3. Simulations of physical systems (Week 12-15)
    - Random Systems: random number generation, random walks, diffusion, cluster growth (Lecture 23)
    - Monte Carlo simulations: integration, importance sampling, Markov chains, Metropolis algorithm (Lecture 24-25)
    - Simulated annealing: function optimization, spin systems, parallel tempering (Lecture 26)
    - Molecular dynamics simulations: Verlet algorithm, atomic collisions (Lecture 27-29)

Remote instruction

This semester, the course will be taught online over Zoom. All lectures and labs will be held synchronously during the designated times. The format will be very similar to an in person class. The lectures and labs will be interactive with opportunity for you to ask questions, write code, and to discuss and collaborate in smaller groups using breakout rooms. I strongly encourage everybody to have their video enabled, if possible. A recording of each Zoom lecture (speaker view) will be provided afterwards. If you have concerns or objections related to the recording, please let me know. All privacy request will be automatically honored. There will also be an online forum where you can post questions and feedback and collaborate with each other.

General office hours will be held virtually under the same Zoom link as the lectures. Additional one-on-one Zoom meetings can be scheduled by appointment. Please do not hesitate to email me if you would like to meet.

Weekly updates and additional course announcements will be posted on Blackboard and sent via email. Please make sure to check your email regularly.

The change to remote instruction is challenging and we will adjust throughout the semester to find a setup that works best for everybody. If you have any questions or concerns, please do not hesitate to reach out. In particular, if you experience problems with access to Zoom or other resources, or any other difficulties related to working from home, please let me know so I can support you.

Book suggestions

There is no required textbook. The course will be self-contained, but you are encouraged to read more about the material in textbooks and to make use of the many available (and free!) online resources, tutorials etc. Specific references and recommendations will be given throughout the course. Here is a list of books that me and others have found useful:

- "Computational Physics" by Mark Newman (guide to Python in computational physics)
- "Numerical Recipes" by W. H. Press *et al.* (covers very comprehensibly a vast range of numerical topics; 3rd edition is in C++; older editions, e.g. in C, are freely available online)
- "Clean Code" by Robert C. Martin (great book on good programming practices)

Lectures

The course lectures will be a combination of lectures on techniques and example programs. You are not expected to have significant expertise with many of the physical examples we will use. Simply try to understand the underlying physics at a low level, and pay attention to how computer techniques open up new levels of understanding.

Labs

The labs will be less formal than the lectures with main focus on hands-on programming. We will also further discuss and review the course material and homework, especially the more difficult topics. You can consult with the instructor and other students on the concepts and problems, or work together on programming. The labs will help you solve the homework assignments.

Computations

Python will be our default programming language, but you may also submit your homework programs in C++ if you prefer. Early work in the labs will help you set up and get familiar with the needed software and tools, and ensure that everyone has a working programming environment.

Homework

There will be weekly homework assignments, which need to be submitted by the deadline via Blackboard. Instructions on the homework submission will be given on the first assignment. In addition, there will be short weekly pre-class warm-up exercises, to be submitted an hour before the first lecture of the week. These will be graded based on (honest) participation only and will help you get prepared for the week's lectures.

Project

The project is an opportunity to apply the methods learned in the course to a physical system that interests you. It will require writing a computer program and presenting the problem, methods, results, and conclusions during the finals slot at the end of the course.

Grading

The course grade will be calculated as follows:

- warm-up exercises: 5%
- homework: 35%
- two exams: 40% (20% each)
- project: 20%

Course grade percentages (may be adjusted):

A: ≥92%	A-: 92%-88%	B+: 88%-84%	B: 84%-80%	B-: 80%-76%	C+: 76%-72%
C: 72%-68%	C-: 68%-64%	D+: 64%-60%	D: 60%-55%	D-: 55%-50%	F: <50%

Accommodations

UMass Boston is committed to providing reasonable academic accommodations for all students with disabilities. Please contact the Ross Center for Disability Services (`ross.center@umb.edu`, 617-287-7430) for recommendations for specific accommodations if needed. If you already have a recommendation, please contact me as soon as possible, preferably within the first two weeks of classes, so that we can work out the best way to support you.

Student mental health

If you or someone you know experiences academic stress, difficult life events, or feelings of anxiety or depression, we encourage you to seek support. Helpful, effective resources are available via the University Health Services. The UHS Counseling Center can be reached at 617-287-5690 (including after-hours and on weekends). Whether or not you are a current patient at the center, you will be able to access telehealth crisis support. Please know that the Counseling Center and university are working to provide remote support for students during this difficult time. More information is available online at
`https://www.umb.edu/healthservices/counseling_center`

Student conduct

Students are required to adhere to the University Policy on Academic Standards and Cheating, to the University Statement on Plagiarism and the Documentation of Written Work, and to the Student Code of Conduct. The Student Code of Conduct and Instructional Setting Conduct Policy are available online.