PHYSIC 362 Computational Science — Spring 2024

Instructor:	Olga Goulko	Lectures:	Tu&Th 2-3:15pm, H03-0009F
Office:	ISC-1-1180	Lab:	Fri 2-3:50pm, H03-0009F
Email:	`olga.goulko@umb.edu`	Homework due:	Fri 2pm
Office hours:	Tu&Th 3:30-4:30pm or by appointment		

This Python-based 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 662. 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 exams are tentatively scheduled during lectures 14 and 29.

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)

Book suggestions

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 and Labs

The course lectures will be a combination of lectures on techniques and example programs. 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. Laboratory and homework will be done on your own laptops or on the computers in lab H03-0009F. Early work in the labs will help you get familiar with the needed software and tools, and ensure that everyone has a working programming environment.

Homework

Doing the homework is the most important aspect of mastering the course material. The only way to learn how to transfer the abstract concepts that we cover in the lectures to practical applications is through solving problems. 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 on Blackboard two hours 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.

You are encouraged to work in groups to figure out how to solve the homework problems. But, you must code and write up your solutions independently. You may not copy another's code or problem solution and present it as your own. **No late assignments will be accepted under any circumstances,** but the worst two assignments will be excluded from your final grade.

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

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 in a poster presentation during the finals slot at the end of the course.

Grading

The course grade will be calculated as follows:

- warm-up exercises: 5%
- homework: 20%
- two exams: 50% (25% each)
- project: 25%

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%

The grade incomplete (INC) can be given only to students in otherwise good standing when a portion of the required class work, or the final examination, has not been completed because of serious illness, extreme personal circumstances, or scholarly reasons at the request of the instructor. Please see www.umb.edu/registrar/policies for additional information, as well as for the pass/fail/withdrawal deadlines.

Academic Integrity and Student Conduct

Education at UMass Boston is sustained by academic integrity, which requires that all members of the campus community are honest, trustworthy, responsible, respectful, and fair in their academic work. 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 via www.umb.edu/academics/academic_integrity.

All of the materials for this course are under copyright, which means that while you are free to download them for your own use as a student in the class, **you may not post online or otherwise circulate outside the class any course materials without the written permission of the instructor**. In particular, you are not allowed to upload any course materials to any academic assistance site such as Chegg. Doing so is against course policy and a violation of copyright, for which you will be legally liable.

I have a zero-tolerance policy for cheating, and all violations will be reported to the University and result in an automatic F grade for the entire course. If you have any doubts or questions about what constitutes academic misconduct, please do not hesitate to contact me.

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