Computer Simulations in Physics

PHYS 338 Spring 2023

Instructor: Katharina Vollmayr-Lee
email: kvollmay@bucknell.edu
Olin 152

Classes: TR 10:00 – 11:20 am RCHM 009

Office Hours: M 2:00–3:00 and F 2:00–4:00 ← This week unusual because I will meet with each one of you individually

webpage: http://www.eg.bucknell.edu/~kvollmay/phys338_s2023/

Texts: (online chapters:) M. Newman, *Computational Physics*, CreateSpace, 2013
and (online:) H. Gould and J. Tobochnik, *An Introduction to Computer Simulation Methods*, 3rd edition, Addison-Wesley, Reading 2006
& Scientific papers & books

See webpage for links
& for Newman Ch 1 see HW1

Course Description: This course is about computer simulations in physics and related fields. During the last 40 years the computer has revolutionized the natural sciences and other disciplines such as economy and ecology. Computers have made it possible to study for example the reasons for traffic jams, stock market crashes, and the shapes of snowflakes. In these and many other examples, a simple rule governs a single element, such as a car, an investor, or a water molecule, which then gives rise to the complex behavior of the system as a whole. The computer takes care of applying the rules to a large number of elements. With computer simulations the models can be tested exactly contrary to experiments where for example impurities might play an additional rule. In nowadays science we use the interplay of theory, experiments and simulations.

- pretty! (playground)
- no impurities (compared to experiment)
- access to analytically not solvable problems (compared to theory)

Objectives: You will learn in this class how to write and run your own Python programs and how to analyze the resulting data. We will start with an introduction to Linux and Python. For the remainder of the course you will learn about modeling (the elements and rules) via the examples listed in the course syllabus below and a project of your own choice. In a more general sense the main goal of this course is to give you an introduction to research by doing it yourself.

Goals: For more general learning goals for physics, astronomy, and biophysics, see
`http://coursecatalog.bucknell.edu/collegeofartsandsciencescurricula/areasofstudy/physicsandastronomy/#goalstext`
For our course the following goals apply:

- "Exhibit a proficiency in the methods of scientific inquiry in laboratory and/or research projects."
- "Present well-organized, logical and scientifically sound oral and written scientific reports."
- "Use critical thinking skills to formulate and solve quantitative problems."

or more specific I hope that you will:

- gain an understanding of modeling and computer simulations in physics and related fields
- learn how to program
- have practiced how to do research
- have gained a deep understanding in one academic research area (and hopefully experiencing the passion for your project)

Course Structure: This course will be a mixture of (mostly) in-class computer lab work, mini lectures, and seminars (given by you!).
There are two components to this course:
1. There are "in-class topics" which will be covered by everybody in class: Intro to Python, Random Walks, Fractal Growth , MD Simulations & Chaos, and Traffic Flow (see syllabus.)
2. Additionally, each of you will have your own semester long "main project."

For the *in-class topics* you will get as preparation for each class homework assignments such as reading assignments with a few questions and/or small programs. Usually at the beginning of class I will give an introduction to the in-class lab work. To be most efficient with our time and to allow for collaboration in this remote class, you will often work in groups of two. At the end of the Fractal Growth, the Chaos, and the Traffic Flow sections you will work on mini-projects I — III (see syllabus.)

For your own semester long *main project* you choose your subject and model, and find and read related scientific literature, write your own program, and analyze the resulting data. You will give two scientific talks. The second talk will be a public symposium talk. To ensure everybody assistance with their project, we will have "individual meetings" (see syllabus), i.e. scheduled office hours, for which everybody will sign up. I encourage your usage of office hours.

Grading: *There will be no exams and no final!* You will have to keep up with the course on a day to day basis, because we will cover a lot of course material in a short amount of time and your main project will require a whole semester's work. Your main project will amount to 67% of your grade, homework and mini-projects account for another 24% and the remaining 9% is for participation.

To maintain the right pace for your *main project* there are various deadlines given in the syllabus and marked with an asterik. You will give two talks. The first will be about the background of your subject and a precise description of the model. A complete description of your project, including model, simulation details, data analysis and conclusions will be in your second talk. Both homework as well as the many different deadlines are implemented to ensure you to be prepared for class and to allow for many different revisions, so for your learning progress. It is therefore essential that you hand in your assignments on time. For occasional super stressful times during the semester you may ask for up to two extensions. Beyond that for any late assignments you will get a 10% point reduction for each late calendar day (maximal reduction: 50%).

Homework assignments have the purpose to prepare you for the in-class work. For the mini-project I you will present your results in a 4 min long talk. Mini-projects II & III will happen in class.

Your participation in this course is essential and therefore 9% of your grade is on *participation*. **Attending and being on-time is mandatory.** Participation also includes working as a team, being prepared for class and class participation. Therefore you may not do phone calls, texting, web-surfing or emailing during class. Attendance and participation are required for the following reasons:

- This is a computer lab course and thus in-class work cannot be made up easily outside of class.
- The course material is cummulative and therefore each class is planned under the assumption that all previous course material is known.
- Some in-class work is covered only in class and not in form of homework, because your homework will often be for your project.
- At the beginning of each class I will give an introduction to the in-class lab work and therefore you have to be on time.
- Sometimes you will work in groups and therefore need to be there as fairness to your classmates.
- Most importantly, these are work place skills you will need after Bucknell.

Grading (continued): If you must miss class (e.g. for a job interview), you must arrange with me ahead of time to make up the missed class. If this is not possible (e.g. last-minute emergencies), you must contact me as soon as reasonably possible so that I can help with planning how to make up any class that you will need to miss.

Participation	9%
Homework	10%
Mini-Projects:	
Project I	6%
Project II	4% } in class
Project III	4%
Main Project:	
Bibliography & Model	9%
Background	4%
First Talk	9%
Flow Chart	7%
2nd Vs. Program	8%
Results	8%
Abstract	4%
Second Talk	9%
Final Program	9%

67 %

Academic Responsibility: You are encouraged to work together on assignments, but the "write up of your solutions" you have to do individually. In the case of programs this means that you have to write the program yourself. There will be a few exceptions in class when you will work in a group. I will clarify thoses cases. In the case of any doubt please ask.

Accommodations: Any student who may need an accommodation based on the impact of a disability, should contact the Office of Accessibility Resources (OAR) at 570-577-1188 or OAR@bucknell.edu. The office will help coordinate reasonable accommodations for those students with documented disabilities. Please visit https:www.bucknell.edu/Accessibility for more information about the OAR.

Inclusive: We will strive for an inclusive classroom as described in The Bucknell University Solidarity Creed (2015)

"As a member of this community, I will respect the diversity of all individuals, including, but not limited to, their sex, gender, identity, expression, race, ethnicity, age, class, citizenship, sexual orientation, nationality, socio-economic status, religion, physical ability and mental ability," the creed reads in part. "I will commit to educating myself about cultures, identities and experiences other than my own."

For resources on diversity see

`https://www.bucknell.edu/life-bucknell/diversity-equity-inclusion`

Covid-19 & Monkeypox: To keep our classroom community safe, please stay home if you are not feeling well or are at an increased risk of carrying COVID, monkeypox, the bubonic plague, or anything else you don't want to pass along to your classmates. In this case, please contact me immediately, via email, office hours, or in your journal entry, so that we can make arrangements.

College in the Wake of a Crisis: We—as individuals, as a university, and as a nation—are in the wake of many crises. A national racial reckoning, a global pandemic, the #metoo movement, a wave of anti-trans legislation, the increase in anti-Asian hate crimes, sharpened anti-Semitism, reduction of women's right, and an uncertain economic future combine to create a time of intense stress and increased anxiety. And everyone will experience different levels of stress and anxiety at different times during the semester. As a class community, I encourage us to collectively move through the semester thoughtfully, kindly, and empathetically. I encourage us to communicate (when necessary and comfortable) with each regarding our health and well-being. And perhaps most importantly, I encourage each of us to prioritize self-care and accountability.

In-Class

Your Main Project

Course Syllabus

Outcomes/Goals
1. Scientific Approach (Your Project)
2. Programming

Date	Topic	Due Dates
Jan. 17	Introduction	individual meetings — See HW 1, 1A find your project
Jan. 19		individual meetings
Jan. 24	Introduction to Python (N Ch 1 & 2)	Bibliography / Model 1st Version*
Jan. 26		
Jan. 31	2. Intro to programming	Bibliography / Model 2nd Version*
Feb. 2	Random Walks (GT Ch 7)	
Feb. 7	Scientific Talks	Bibliography / Model Final Version*
Feb. 9		
Feb. 14	Fractal Growth (GT Ch 13)	Flow Chart 1st Version*
Feb. 16		Background 1st Version* ← 1B become expert
Feb. 21		Talk Slides 1st Version* (Backgr. Final Vs.)*
Feb. 23		Program 1st Version* ← 1D write Program
Feb. 28	Mini-Project I	Mini-Project I
March 2	Talks I (Main Project)*	1C Talks
March 7		Flow Chart Final Version*
March 9	I will be at Conference — MD Simulations	Program 2nd Version*
March 21	Chaos (GT Ch 4–6)	
March 23		Program 3rd Version*
March 28	Mini-Project II	Results 1st Version*

main project deadlines to help you stay on track

Date	Topic	Due Dates
March 30	Your Project (in class)	Results 2nd Vs*
April 4		
April 6		Final Program*
April 11	Traffic Flow	
April 13		Results Final Version*
April 18	Mini-Project III	Abstract (IE write abstract)
April 20	Summary & Outlook	Talk Slides 1st Version*
April 25	Symposium Talks II*	
April 27		