Computer Simulations in Physics

PHYS 338   Spring 2021

Instructor: Katharina Vollmayr-Lee
email: kvollmay@bucknell.edu
less under Covid-19:
152 Olin
office phone: 577-3109

Classes: TR 10:20 – 11:40 am   Zoom ID 97645789035 Passcode 808111

`https://bucknell.zoom.us/j/97645789035?pwd=cnVTNnh3S29iNXNTT3FqQzFSMTdxUT09`

Office Hours: Tentative: M 2:00–3:30, T 4:30–5:30, and F 10:30-12:00

webpage: http://www.eg.bucknell.edu/~kvollmay/phys338_s2021/

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

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.

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 (remotely) 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 , 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 write two scientific papers and you will give two scientific talks. The second talk will be a public conference talk. I will make a pamphlet with your abstracts for this conference. 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 72% of your grade, homework and mini-projects account for another 19% 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 write two papers and 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 paper and 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 write a one page long paper and you will present your results in a 3 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 includes working as a team, being prepared for class and class participation. During class time I expect your full attention. This will be particularly difficult since we meet remotely, i.e. the distractions are even more difficult to avoid. Attendance and your full 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 meetings.
- 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.
- These are work place skills you will need after Bucknell.

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.

Grading (continued):	Participation	9%
	Homework	9%
	Mini-Projects:	
	Project I	4%
	Project II	3%
	Project III	3%
	Main Project:	
	Bibliography & Model	8%
	Background & Methods	8%
	First Paper	8%
	First Talk	8%
	Flow Chart & 1st Vs. Program	8%
	Results & Abstract	8%
	Second Paper	8%
	Second Talk	8%
	Final Program	8%

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: If you have a disability that may have some impact on your work in this class and for which you may require accommodations, please contact me and please contact the OAR at OAR@bucknell.edu; 570-577-1188 or complete the Disability Accommodation Request form (https://bucknell-accommodate.symplicity.com/public_accommodation/). The OAR will coordinate reasonable accommodations for students with documented disabilities.

Inclusive: We will strive for an inclusive classroom as described in The Bucknell University Solidarity Creed
`https://bucknellian.net/53883/news/solidarity-ceremony-calls-for-change/`
"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."

and as described in Bucknell's Diversity, Equity, And Vision & Statement
`https://www.bucknell.edu/life-bucknell/diversity-equity-inclusion`

Course Syllabus

Date	Topic	Due Dates
Feb. 2	Introduction	individual meetings
Feb. 4	Introduction to Python (N Ch 1 & 2)	individual meetings
Feb. 9		Bibliography / Model 1st Version*
Feb. 11		
Feb. 16		Bibliography / Model Final Vs.*
Feb. 18	Random Walks (GT Ch 7)	
Feb. 25	Paper Wr. Tools	Background & Methods*
March 2		
March 4	Fractal Growth (GT Ch 13)	1st Paper: 1st Version*
March 9		
March 11	Talk Tools	1st Paper: Final Version*
March 16	Mini-Project I	Mini-Project I
March 18	Talks I	Flow Chart 1st Version*
March 23		
March 25	Your Project (in class)	Program 1st Version*
March 30		Flow Chart Final Version*
Apr. 1	MD Simulations	Program 2nd Version*
Apr. 6	& Chaos (GT Ch 4–6)	Program 3rd Version*
Apr. 8	Mini-Project II	

Date	Topic	Due Dates
Apr. 13	Mini-Project II (continued)	Results 1st Vs* (Figs. & Interp.)
Apr. 15	Figures & Your Project	Results 2nd Vs* (Figs. & Interp.)
April 20	Traffic Flow	Final Program*
April 27		Results (Sect. of Paper)*
April 29		Abstract*
May 4	Mini-Project III	
May 6	Symposium: Talks II	2nd Paper: 1st Version*
May 10		
May 12		
May 18 6:30pm (Final)		2nd Paper: Final Version*