Computer Simulations in Physics

PHYS 338 Spring 2017

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Classes: TR 9:30 – 11 am ACWS 204

Office Hours: WF 1–2, MWF 2–3 and by appointment

webpage: http://www.eg.bucknell.edu/~kvollmay/phys338_s2017/

Texts: M. Newman, *Computational Physics*, CreateSpace, 2013
and (online:) H. Gould and J. Tobchnik, *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.

For more general learning objectives see
http://www.bucknell.edu/x50075.xml

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 , 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 as practice for team work, you will sometimes 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. We will make a pamphlet with the 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 62% of your grade, homework and mini-projects account for another 28% and the remaining 10% is for professionalism.

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. For any late assignments you will get a 10% point reduction for each late calendar day (maximal reduction: 50%).

Since the *homework* assignment has the purpose to prepare you for the in-class work, you will get **no** credit for any late homework assignment. For the mini-project I you will write a two page long paper and you will present your results in a 5 min long talk. Mini-projects II & III will happen in class.

Grading (continued):

Your participation in this course is essential and therefore 10% of your grade is on *professionalism*. **Attending and being on-time is mandatory**. Professionalism 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.
- 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.

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.

You are encouraged to work together on homework, 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. For further clarification of academic responsibility please see `http://www.bucknell.edu/x1324.xml` and `http://www.bucknell.edu/Documents/Engineering/ComputerScience/student-conduct-policy.pdf`. In the case of any doubt please ask.

Professionalism	10%
Homework	10%
Mini-Projects:	
Project I	8%
Project II	5%
Project III	5%
Main Project:	
Bibliography & Model	5%
Background & Methods	5%
First Paper	8%
First Talk	8%
Flow Chart & 1^{st} Vs. Program	5%
Results & Abstract	5%
Second Paper	8%
Second Talk	8%
Final Program	10%

Course Syllabus

Date	Topic	Due Dates
Jan. 17	Introduction	individual meetings
Jan. 19	Introduction to Python (N Ch 2 & 3)	individual meetings
Jan. 24		Bibliography / Model 1st Version*
Jan. 26		
Jan. 31		Bibliography / Model Final Vs.*
Feb. 2	Random Walks (GT Ch 7)	
Feb. 7	Paper Wr. Tools	Background & Methods*
Feb. 9		
Feb. 14	Fractal Growth (GT Ch 13)	1st Paper: 1st Version*
Feb. 16		
Feb. 21	Talk Tools (N Ch 3)	1st Paper: Final Version*
Feb. 23	Mini-Project I	Mini-Project I
Feb. 28	Talks I	Flow Chart 1st Version*
March 2		individual meetings
March 7	Your Project (in class)	Flow Chart Final Version*
March 9		Program 1st Version*
March 21	MD Simulations	
March 23	& Chaos (GT Ch 4–6 & N Ch 8)	Program 2nd Version
March 28	Mini-Project II	

Date	Topic	Due Dates
March 30	Your Project (in class)	Results (Figures & Interpret.)*
April 4		
April 6	Traffic Flow	Final Program*
April 11		Results (Sect. of Paper)*
April 13	Mini-Project III	Abstract*
April 18	Summary & Outlook	
April 20		2^{nd} Paper: 1^{st} Version*
April 25	Symposium: Talks II	
April 27		
May 9, 9:30am (Final)		2^{nd} Paper: Final Version*