# Computer Simulations in Physics

**PHYS 338 Spring 2019**

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**Classes:** TR 9:30 – 11 am RCHM 009

**Office Hours:** MWF 2–3, T 4–5 and by appointment

**webpage:** http://www.eg.bucknell.edu/~kvollmay/phys338_s2019/

**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

— see links on web page & scientific papers etc.

**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.

(playground)
- no impurity
- access to analytically not solvable problems

**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 , Chaos, and Traffic Flow (see syllabus.)
2. Additionally, each of you will have your own semester long "main project."

see syllabus

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. 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.

HW#1 ←

**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 64% of your grade, homework and mini-projects account for another 27% and the remaining 9% 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 6 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 *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.
- 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.

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):**

| | |
|---|---|
| Professionalism | 9% |
| Homework | 9% |
| Mini-Projects: | |
| Project I | 8% |
| Project II | 5% } in class |
| Project III | 5% } in class |
| Main Project: | |
| Bibliography & Model | 6% |
| Background & Methods | 6% |
| First Paper | 8% |
| First Talk | 8% |
| Flow Chart & 1st Vs. Program | 6% |
| Results & Abstract | 6% |
| Second Paper | 8% |
| Second Talk | 8% |
| Final Program | 8% |

64 %

**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. For further clarification of academic responsibility with respect to programming please see `http://www.bucknell.edu/x1324.xml` and responsibility with respect to programming please see the policy extension described by the computer science engineering department `http://www.bucknell.edu/Documents/Engineering/ComputerScience/student-conduct-policy.pdf`. 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 see me and Heather Fowler, Director of the Office of Accessibility Resources at hf007@bucknell.edu, 570-577-1188 or in room 107 Carnegie Building so that such accommodations may be arranged.

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

`http://www.bucknell.edu/news-and-media/2015/april/standing-in-solidarity.html`

"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/about-bucknell/diversity-equity-and-inclusion-at-bucknell/diversity-equity-and-inclusion-vision-and-statement`

# Course Syllabus

In-Class

Main Project *

| Date | Topic | Due Dates |
|---|---|---|
| Jan. 15 | Introduction | individual meetings |
| Jan. 17 | Introduction to Python (N Ch 1 & 2) | individual meetings |
| Jan. 22 | | Bibliography / Model 1st Version* |
| Jan. 24 | | |
| Jan. 29 | | Bibliography / Model Final Vs.* |
| Jan. 31 | Random Walks (GT Ch 7) | |
| Feb. 5 | Paper Wr. Tools | Background & Methods* |
| Feb. 7 | | |
| Feb. 12 | Fractal Growth (GT Ch 13) | 1st Paper: 1st Version* |
| Feb. 14 | | |
| Feb. 19 | Talk Tools | 1st Paper: Final Version* |
| Feb. 21 | Mini-Project I | Mini-Project I |
| Feb. 26 | Talks I (Main Project)* | Flow Chart 1st Version* |
| Feb. 28 | Your Project (in class) | Program 1st Version* & individual meetings |
| March 5 | | Flow Chart Final Version* |
| March 7 | | Program 2nd Version* |
| March 19 | MD Simulations | |
| March 21 | & Chaos (GT Ch 4–6) | Program 3rd Vs & Results 1st Vs* |
| March 26 | Mini-Project II | |

see HW1 (webpage sign-up link) You choose subject for your project

see hand-out

main project deadlines to help you staying on track etc.

at beginning:
- start project
- linux (HW#1)
- python (start Thu)

| Date | Topic | Due Dates |
|---|---|---|
| March 28 | Your Project (in class) | Results 2nd Vs* |
| April 2 | | |
| April 4 | | Final Program* |
| April 9 | Traffic Flow | Results (Sect. of Paper)* |
| April 11 | | Abstract* |
| April 16 | Mini-Project III | |
| April 18 | Summary & Outlook | 2nd Paper: 1st Version* |
| April 23 | Symposium Talks II* | |
| April 25 | | |
| TBA (Final) | | 2nd Paper: Final Version* |

# Literature Search

**Goal:** For now our goal is that you find the topic and specific model for your main project. (Only later your goal will also be to become an expert, i.e. to know related previous work.) Find model simple enough, yet some rules to program. Look for sources (papers/books) and check whether they are well written. Can you follow their description of the "rules of the game". For example for a traffic flow model on lattice: Which lattice, how do velocities and positions get updated at each time step?

**Outline:**

Go to our PHYS 338 webpage
`http://www.eg.bucknell.edu/~kvollmay/phys338_s2019/`
and scroll down to "Guidelines For Main Project" and "Literature Search Tools". I will guide you through the provided links and you will get to practice them with topics which sparked your interest.

## 1. Links on PHYS 338 webpage

I will give you a quick guide through the links of the PHYS 338 webpage.

### Guidelines For Main Project:

- Previous simulation projects: These are the posters for the symposia, so talk titles of main projects students chose in previous years. You may use these posters to see examples for a wide range of topics.
- Traffic Flow Paper: We will use this paper for our last in-class topic. It is a great example for a well written paper with also many references for other models.(more details in later classes of our courses)
- Computational Physics Section of AJP (eidtors Gould & Tobochnik). This selection of papers is intended for undergraduate and graduate students to provide an introduction is a variety of topic in computational physics.
- Bibliography/Model: Assignment for Jan.22. I will walk you through this assignment in more detail in next class.

### Literature Search Tools:

- Web of Science and Google Scholar are for finding papers. This is your main tool kit.
- Library & IT is the top page, from which you can get to all other pages. Here you find also `Interlibrary Loan` (ILL) which you need for getting papers or books,to which Bucknell does not have access to.
- Databases includes Web of Science and other Databases for humanities and social science papers. Use this link when you try to use Web of Science from outside of Bucknell.
- Book: BU Library Catalog (World Cat). This is for finding books at Bucknell and also at other libraries.

- The physics resources are for some specific journals which you most likely will need and also the preprint server arXiv.

**2. Web of Science**

Click on the Web of Science link. (In case you are using Web of Science while not being directly on the Bucknell internet, you can get into Web of Science by using the Databases link and then Web of Science, which will ask you for your Bucknell login information.) Below a list I will guide you through:

- Start with "Basic Search"
- Add Another Row ; Topic or other setting
- Search by topic (e.g. Ising Model or any other topic)
- refine search (e.g. ising ferromagnet and simulation)
- click on title $\rightarrow$ Cited References (Past)
- Times Cited (Future) (more recent papers have fewer citations).
- View Related Records
- get paper via `Full Text from Publisher` or via `Links`
- to get paper via ILL, if Bucknell has no access to it, use `Links` then `GET IT`. (add to the ising ferromagnet and simulation search also `Ozkan` as author and click on the result Phase transitions, volume 89, pages 94-105, 2016)
- take notes in extra file to keep the information about good papers and also which keywords worked and which not
- search by author if you found well written papers by specific author
- search by year if you look for specific paper or if you e.g. want to search for more recent papers only.