# SYLLABUS

## PHY411/PHY506: Computational Physics 2

Hours: **MWF 2-2:50 PM** Classrooms: **Fronczak 219**
Instructor: Dr. Salvatore (Sal) Rappoccio Office: 335 Fronczak
Phone: 645-6250 E-mail: srrappoc@buffalo.edu
Office Hours: Tues 9-10, Wed 3-4, and by appointment

This course is the second in a sequence of two courses in Computational Physics that integrates numerical analysis and computer programming in C++ and python (and their combination), to study a variety of problems in physics. (1) Partial Differential Equations, (2) Probabilistic Methods, (3) Quantum MC methods, (4) Proteins and Neurons, (5) Machine Learning. There will also be a required coding project that will take at least a month of time.

PREREQUISITES AND BASIC RESOURCES:
You are required to have taken PHY 410/505 or equivalent, and have familiarity with the C++ and python programming languages. This course assumes familiarity with undergraduate physics at the junior/senior level. You should have passed PHY 301, PHY 401, and PHY 403, or equivalent courses, or be taking them concurrently. If you are not a physics major, a strong background in undergraduate mathematics or computer science should suffice if you spend extra time to learn the physics background required for each topic, although you should be familiar with ordinary and partial differential equations at the very least.

Familiarity with a modern programming language is required (C++/Java/Fortran/`python`/etc). Programming mainly with C++ and `python` will be covered in the first 4-8 weeks of lecture. If you are not familiar with C++ or `python` you should spend extra time very early in the course to bring yourself up to speed. Depending on experiences of the class, we will spend more or less time on introductions to programming. We will discuss how to compile and execute your code on your chosen platform. For instance, it will be helpful to have familiarity with `bash`, `tcsh`, or `zsh` for Linux/Unix/Macintosh, or `cygwin` for Windows. We will discuss how to combine C++ and `python` with existing tools such as SWIG.

REQUIRED MATERIALS:

Personal laptops are recommended for this class. The primary method of distribution of software is via Docker container, so please ensure you can use docker if you use a personal laptop. Alternatively you can use Windows with cygwin, Macintosh (OS X 10.5 or later), or Linux (e.g. Ubuntu). All required software for this course can be downloaded for free. Detailed lecture notes and online references will be provided. The Windows 10 operating systems may use the bash shell functionality.

The required textbooks are required (and free of charge). You are expected to have working knowledge of things covered in these books.

- Fundamentals of C++ Programming by Richard Halterman
    - Example code at https://github.com/halterman/CppBook-SourceCode
- https://www.tutorialspoint.com/python3/ : Introduction to python
- Numerical Recipes in C++ :
    - The latest version **does cost money** but is a worthwhile investment for your career, while **older versions of NR are free.**
    - Earlier online version of NR for free

The following are also helpful resources:

- http://www.physics.buffalo.edu/phy410-505/ Previous years' course site
- Programming - Principles and Practice Using C++ by Stroustrup
- http://www.python.org Python programming language official website
- http://www.swig.org : SWIG for combining C++ and python
- Numerical Methods for Physics by Alexander Garcia

The course website is at UBLearns :

- http://ublearns.buffalo.edu/ UBLearns course site

Editors :

- http://www.gnu.org/software/emacs/ : emacs
- http://www.vim.org : VIM
- https://developer.apple.com/xcode/ : XCode

Version Control Software :

- http://github.com : git

Containers:

- https://www.docker.com: docker

SCHEDULE:

The course is scheduled MWF 2-2:50 PM. Homework will be regularly assigned (~weekly). There is a take-home midterm and final project.

EXPECTATION

To succeed in this course you should read the lecture notes and posted materials, attend class and participate actively in discussion and quizzes, complete the homework assignments on time, and take the midterm and final exams. Exceptions will be made for documented medical reasons or major emergencies.

If you are having difficulty with the course material, it is best to be proactive and contact me directly, either in office hours or by appointment. Discussing difficulty beforehand is encouraged, but asking for special consideration after the fact is not usually helpful.

GRADING:

Grades will be based on your scores on homework (50%), one take-home midterm (25%), and a final project (25%). Graduate students and undergraduates will be graded separately.

The lowest homework score will be dropped from consideration to accommodate personal situations such as illnesses or missed classes.

**MIDTERM:** Mid-semester (Take home)

**FINAL PROJECTS AND PRESENTATION:** During the last 1-2 months of classes, you will be required to perform a project of your own choosing using the techniques developed in class. You will also be required to give a 15-minute presentation on your work during the last two weeks of classes. We will draw a random lottery at the start of each class to see who gives the presentations to ensure everyone has the same amount of time to work on their projects and presentations. You are also required to attend the presentations of your peers to support and encourage them.

ACADEMIC INTEGRITY

Academic integrity is a core value underlying all scholarly activity in the Department of Physics. Please review UB undergraduate policy at http://undergrad-catalog.buffalo.edu/policies/course/integrity.shtml or graduate policy in http://www.grad.buffalo.edu/policies/academic_integrity.pdf. You are encouraged to discuss class material and assignments with your colleagues (with acknowledgment of who you worked with on your assignment). However, you should code and run your simulations yourself, and your homework writeup must be entirely your own effort. If you copy and/or modify code from any source for your assignments you should acknowledge this with an appropriate citation in your writeup.

STUDENTS WITH DISABILITIES

If you have a disability, (physical or psychological) and require reasonable accommodations to enable you to participate in this course, such as note takers, readers, or extended time on exams and assignments, please contact the Office of Disability Services, 25 Capen Hall, 645-2608, http://www.student-affairs.buffalo.edu/ods/, and also see me me during the first two weeks of class. ODS will provide you with information and review appropriate arrangements for reasonable accommodations.

# Learning Outcomes

| TOPIC UNITS | LEARNING OUTCOMES | OUTCOME ASSESSMENT |
|---|---|---|
| Partial differential equations | Elliptic, parabolic and hyperbolic equations, Poisson's equation in electrostatics, wave motion, spectral methods, quantum wavepacket motion. [U:2,5] [G:3,4,5] | Homework, midterm, projects |
| Probabilistic methods | Random numbers, random walks, polymer dynamics, the Metropolis algorithm, Monte Carlo simulation of the hard disk gas and the Ising model [U:2,5] [G:3,4,5] | Homework, midterm, projects |
| Advanced differential equations with probabilistic methods | Fluid dynamics, Numerical general relativity, [U:3,5,6] [G:2,4,5] | Homework, projects |
| Advanced quantum mechanical methods | Variational MC, diffusion MC, path integral MC, VEGAS algorithm [U:3,5,6] [G:2,4,5] | Homework, projects |
| Proteins and neurons | Protein folding, Hodgkin-Huxley equations, genetic algorithms [U:3,5,6][G:2,4,5] | Homework, projects |
| Advanced data analysis | Kalman filters, K-means clustering, the inverse problem, regression [U:3,5,6] [G:2,4,5] | Homework, projects |
| Machine learning | Artificial neural networks, decision trees, deep neural networks [U:3,5,6] [G:2,4,5] | Homework, projects |

The "U" (undergraduate) bracketed numbers in the 2nd column give the correspondence to the Physics Department's undergraduate curriculum goals: [1] The basic laws of physics; [2] Critical thinking and problem solving; [3] Laboratory skills; [4] General knowledge of the development of physics; [5] Contemporary areas of physics inquiry; [6] Written and oral communication skills. Note that not all courses emphasize all of the above goals.

The "G" (graduate") bracketed numbers in the 2nd column give the correspondence to the Physics Department's graduate curriculum goals: [1] The basic laws of physics; [2] Advanced knowledge in a specialty area; [3] Broad knowledge of physics topics outside the specialty area; [4] In-depth scientific research skills; [5] Teaching and communication skills. Note that not all courses emphasize all of the above goals.