PHY 371

Introduction to Programming for Computational Sciences Fall Semester, 2014

Instructor: Dr. Ying Tang **Office**: KOS 236

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Office Hours: Monday 8:00am – 10:00am, Tuesday 10:00am–12:00pm

Wednesday 10:00am–12:00pm; other times by appointment

Lectures: Tuesday and Thursday 8:00am-9:35pm in KOS 118

Description:

This project-based course is designed to provide students with the objective-oriented programming skills and computational techniques needed for continued studies in computational science and engineering. There are 8 scientific (and fun) projects (6 regular projects, 1 midterm and 1 final project).

Prerequisites:

Introductory Physics I (PHY121) is required. If you haven't taken PHY121 or the equivalent, please come see me at your earliest convenience. Any prior programming experience will be helpful but not required.

Recommended Textbook:

Computational Physics by Mark Newman (Amazon prime)

http://www-personal.umich.edu/~mejn/computational-physics/

References:

- A Survey of Computational Physics by Rubin Landau, et al. (Free online!)
- Python for Data Analysis: Data Wrangling with Pandas, NumPy, and IPython by Wes McKinney
- Annotated Algorithms in Python: with Applications in Physics, Biology, and Finance by Dr Massimo Di Pierro

Objectives:

By the end of the course, students should be able to:

- Program in Python
- Understand the concepts of "objects" and use objected-oriented programming (OOP) constructs and approaches in Python
- Carry out basic operations in Linux
- Use Latex for scientific reports
- Use online version control Github
- Visualize their data

- Analyze data using curve fitting and error analysis
- Perform numerical integration
- Compute the classical equation of motion (differential equations)
- Understand the random walk model and probability distributions
- Program basic cellular automata problems
- Understand the Ising spin model
- Know the basic simulated annealing algorithm
- Develop good presentation skills

Evaluation:

The final grade will be based on the weighted items as shown below:

• Project I – VI: 60 %

• Midterm Presentation: 15 %

• Final Presentation: 15 %

• Peer review on the midterm: 5%

• Peer review on the final: 5%

Grading Rubric (on a scale of 10):

- 10 Extra neat, correct, concise and well-commented code, demonstrate the understanding of concepts in depth.
- 8 Complete and correct. The report includes the analysis of the problem, the program, answers to the questions, and plots.
- 6 Contains a few mistakes but in general is okay.
- 4 Only partially finishes the project or has major mistakes.
- 2 Far from complete.
- **0** No attempt.

You are expected to use Latex to finish your report. Program and report should be submitted to *Github* before the deadline. Late submissions will immediately result in a deduction of 50% of the project credit.

Useful links/software:

Check your grades and course materials at Blackboard: https://blackboard.gordon.edu

Unix Tutorial: http://www.doc.ic.ac.uk/~wjk/UnixIntro/

Official Python Tutorial: https://docs.python.org/2/tutorial/introduction.html

Free online version control (Github): https://github.com

*Have more coding practice at: www.codecademy.com

* Fun python projects I: http://projecteuler.net/problems

*¹Fun Python projects II: http://puzzles.bostonpython.com

Course Policy

 $^{\rm 1}$ A surprise might be given to those who did some extra projects here.

Attendance:

Attendance will be recorded and unexcused absences in excess of 3 occurrences will reduce your total grade.

Academic Dishonesty:

"Academic dishonesty is regarded as a major violation of both the academic and spiritual principles of this community and may result in a failing grade or suspension. Academic dishonesty includes plagiarism (see Plagiarism in Student Handbook), cheating (whether in or out of the classroom), and abuse or misuse of library materials when such abuse or misuse can be related to course requirements." Please note that, you are encouraged to discuss general approaches to solve a problem or share your knowledge with others, etc. However, all your programs and reports should be your original work.

Library Resources:

"Students are responsible to obtain any library resources assigned for this course. Questions about library resources should be directed to librarians in the Jenks Library. Librarians are available to assist you from the library reference desk, by e-mail at library@gordon.edu, or by phone (978) 867-4878."

Students with Disabilities:

Gordon College is committed to assisting students with documented disabilities (see Academic Catalog Appendix C, for documentation guidelines). A student with a disability who may need academic accommodations should follow this procedure:

Meet with a staff person from the Academic Support Center (Jenks 412, Ext. 4746) to:

- make sure documentation of your disability is on file in the ASC,
- discuss the accommodations for which you are eligible,
- discuss the procedures for obtaining the accommodations, and
- obtain a Faculty Notification Form.

Deliver a Faculty Notification Form to each course professor *by Friday, September 5;* at that time make an appointment to discuss your needs with each professor. Failure to register in time with your professor and the ASC may compromise our ability to provide the accommodations. Questions or disputes about accommodations should be immediately referred to the Academic Support Center. See Grievance Procedures available from the ASC.

Academic Support:

There are a variety of resources on Gordon campus for students to search for academic help. Please contact me as soon as you recognize that you are having difficulty with this course or realize you are not effectively working toward your goals for the course.

Evaluation:

Grades will be based on the scale as follows: (minimum percentage, letter grade):

93% A	90% A-	86% B+	83% B	80% B-	76% C+
73% C	70% C-	66% D+	63% D	60% D-	<60% F

(Tentative) Schedule

R 8/28 Course Introduction

Project I: Rock-Paper-Scissors-Lizard-Spock (Due 9/14) + Practice on Codecademy				
<u>Date</u>	<u>Programming</u>	<u>Methods</u>	<u>Sciences</u>	
T 9/2 R 9/4	Introduction to Linux, version control, Python, Latex and other Software			
T 9/9 R 9/11	Variables, Statements, Function, Packages (Numpy, Scipy and Matplotlib)			

Project II: Plotting with Python (Due 9/21) + Keep practicing on Codecademy				
<u>Date</u>	Programming	<u>Methods</u>	<u>Sciences</u>	
T 9/9 R 9/11	Packages (Numpy, Scipy and Matplotlib) continued, Loops, Conditionals, Data type			

Project III: Finding the best fit (Due 9/28)				
<u>Date</u>	<u>Programming</u>	<u>Methods</u>	<u>Sciences</u>	
T 9/16 R 9/18	Loops, Conditionals, Data type	Optimization	Measurements and errors	

Project IV: How much work has been done? (Due 10/5)				
<u>Date</u>	<u>Programming</u>	<u>Methods</u>	<u>Sciences</u>	
T 9/23 R 9/25		Integral methods and Error analysis	Energy and Work	
T 9/30 (No class on 10/2 Day of Prayer)	Introduction to Classes, Encapsulation, Inheritance and Polymorphism			

Midterm Project: Lunch a rocket (Present in class on 10/21 and 10/23)				
<u>Date</u>	<u>Programming</u>	<u>Methods</u>	<u>Sciences</u>	
T 10/7 R 10/9	Practice things learned above	Numerical Differentiation and	Newton mechanics	
		Error analysis		

T 10/14(Quad Break) and R 10/16(Quad Final), no class

T 10/21 R 10/23	Midterm Presentation
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Project V: Cellular Automata (Due 11/11)				
<u>Date</u>	<u>Programming</u>	<u>Methods</u>	<u>Sciences</u>	
T 10/28 R 10/30	Practice recursion and object programming		Cellular Automata	
T 11/4 and R 11/6	Practice recursion and object programming		Cellular Automata and gaming rules	

Project VI: Nuclear Decay (Due 11/18)				
<u>Date</u>	<u>Programming</u>	<u>Methods</u>	<u>Sciences</u>	
T 11/11 R 11/13		Monte Carlo	Nuclear Decay	

Final Project: Choose your own topics (Present in class on 12/2 and 11/6)				
<u>Date</u>	<u>Programming</u>	<u>Methods</u>	<u>Sciences</u>	
T 11/18 R 11/20		Monte Carlo	Magnetism and Spin Models	
T 11/25 (11/26-11/28, Thanksgiving)			Magnetism and Spin Models	
T 12/2 R 12/4	Final project discussion			
T 12/9 R12/11	Final project presentation			