Universidad de Puerto Rico, Recinto de Río Piedras
Facultad de Ciencias Naturales, Departamento de Física

Título: **Tópicos Especiales en Física I: Introduction to Scientific Computing**
Código: PHYS 4041
Créditos: 3
Profesor: **Julian Velev**
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Hours: Mon & Wed 10:00-11:20am; C-312
Office hours: Mon & Wed 11:30-12:30pm or by appointment; C-346

Prerequisites: Sufficient preparation in calculus and physics to understand the examples. Basic computer literacy such as text editing, administering the computing environment (installing applications and libraries), executing code from the command prompt, etc. Access to a computer where the Python programming environment and libraries could be installed (preferably a laptop). It is the students' responsibility to setup their own working Python environment.

Course description: The goal of this course is to develop basic programming proficiency for science majors. In class the students will learn the main programming paradigms: data representation (data types and data structures), program control (branching and loops); input and output (files and visualization); error handling (exceptions); and the basics of object-oriented programming (classes).
This will be done in the context of examples taken from mathematics, physics, biology, and economics. The unifying theme of the examples is that they are statistical in nature. They include numerical methods such as Monte Carlo integration, Monte Carlo simulations of thermodynamic equilibrium, game theory and evolutionary game theory. The students will immediately apply the concepts by implementing the examples in class and also developing applications at home as homework.
The course will use the Python programming language because of its remarkable power coupled with very clean and concise syntax. Python shortens the learning curve allowing the students to quickly progress to the stage of producing meaningful applications. At the same time is a very good foundation for those who will continue to use other programming languages such as C++, Java, and Fortran.

Textbooks:
(1) H. P. Langtangen, *A primer on scientific programming with Python*, 5nd edition, (Springer, 2016), ISBN 978-3662498866;
(2) H. P. Langtangen, *Python scripting for computational science*, 3nd edition, (Springer, 2009), ISBN 978-3540739159

Tentative schedule:

Topic	Title	Reading	Date
0	**Preliminaries** Setup working python environment		Jan 27,29
1	Introduction: **General introduction to computing** *Hands on: Setup the Python environment. First program*	1.1,2	Feb 3,5
2	Data structures: **Variables. Operators. Standard data types. Math library** *Hands on: Celsius-Fahrenheit conversion; Ball thrown vertically*	1.1,3,6; 6.3	Feb 10,12
3	Program elements: **Branching. Loops** *Hands on: Calculation of functions using Taylor expansions*	3.2; 2.1	Feb 19,24
	Assignment 1 (due Feb 24)		
4	Data structures: **Tuples and lists** *Hands on: Celsius-Fahrenheit (table)*	2.2-5; 6.2	Feb 26,Mar 4
5	Data structures: **Arrays, strings, and dictionaries. NumPy library** *Hands on: Polynomial evaluation*	5.1,2,5,6	Mar 9,11
6	Program elements: **Functions. Modules** *Hands on: Numerical differentiation. Interest rates.*	1.4; 3.1; 4.4	Mar 16,18
	Assignment 2 (due Mar 18)		
7	Input/Output: **Standard input/output. Command line. Files** *Hands on: Stock returns*	6.1,5; 5.3,4	Mar 25,30
8	Input/Output: **Visualization. Matplotlib library** *Hands on: Normal distribution. Stock returns (plots)*		Apr 1,6
9	Error handling: Exceptions *Hands on:*	4.3	Apr 13,15
	Assignment 3 (due Apr 15)		
10	Numerical methods: **Random numbers** *Hands on: Uniform and normal distribution histogram*	8.1-3	Apr 20,22
11	Applications: **Monte Carlo sampling** *Hands on: Numerical integration. Monte Carlo integration*	8.5	Apr 27,29
12	Applications: **Metropolis Monte Carlo. Importance sampling** *Hands on: Ising model*	8.6,7	May 4,6
13	Applications: **Game theory. Evolutionary game theory** *Hands on: Cournot duopoly. Hawk-dove game*		May 11,13
	Assignment 4 (due May 13)		

Grading: The grade will be based on four homework assignments, each contributing 25% of the grade. Collaboration on the assignments is not allowed unless the project is explicitly assigned to a group. All assignments will require the student to produce working codes. The assignments should be submitted in a report form with introduction, design, implementation and results sections. The grading scheme is A, B, C, D, F.

University policies:

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