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
Número de Créditos: 3
Profesor: Julian Velev

Hours: Mon, Wed 10:00-11:20; C-312

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.

Topics:

Topic	Title	Reading	Date
1	Introduction: **General introduction to computing** *Hands on: Setup the Python environment. First program*	1.1,2	Jan 20, 25,27
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 1,3

3	Program elements: **Branching. Loops** *Hands on: Calculation of functions using Taylor expansions*	3.2; 2.1	Feb 8,10
	Assignment 1 (due Feb 17)		
4	Data structures: **Tuples and lists** *Hands on: Celsius-Fahrenheit (table)*	2.2-5; 6.2	Feb 17,22
5	Data structures: **Arrays, strings, and dictionaries. NumPy library** *Hands on: Polynomial evaluation*	5.1,2,5,6	Feb 24,29
6	Program elements: **Functions. Modules** *Hands on: Numerical differentiation. Interest rates.*	1.4; 3.1; 4.4	Feb 29, Mar 2
	Assignment 2 (due Mar 9)		
7	Input/Output: **Standard input/output. Command line. Files** *Hands on: Stock returns*	6.1,5; 5.3,4	Mar 7,9
8	Input/Output: **Visualization. Matplotlib library** *Hands on: Normal distribution. Stock returns (plots)*		Mar 14, 16,28
9	Error handling: Exceptions *Hands on:*	4.3	Mar 30
	Assignment 3 (due Apr 4)		
10	Numerical methods: **Random numbers** *Hands on: Uniform and normal distribution histogram*	8.1-3	Apr 4, 6,11
11	Applications: **Monte Carlo sampling** *Hands on: Numerical integration. Monte Carlo integration*	8.5	Apr 13, 18,20
12	Applications: **Metropolis Monte Carlo. Importance sampling** *Hands on: Ising model*	8.6,7	Apr 25, 27, May 2
13	Applications: **Game theory. Evolutionary game theory** *Hands on: Cournot duopoly. Hawk-dove game*		May 4, 9,11
	Assignment 4 (due May 11)		

Textbooks:

(1) H. P. Langtangen, *A primer on scientific programming with Python*, 4nd edition, (Springer, 2014), ISBN 978-3642549588;

(2) H. P. Langtangen, *Python scripting for computational science*, 3nd edition, (Springer, 2009), ISBN 978-3540739159

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.

Accommodation of students with disabilities:
Los estudiantes que requieren acomodo razonable o reciben servicios de Rehabilitación Vocacional deben comunicarse con el profesor al inicio del semestre para planificar el acomodo y equipo necesario conforme a las recomendaciones de la oficina que atiende los asuntos para personas con impedimentos en la unidad.

Academic integrity:
La Universidad de Puerto Rico promueve los más altos estándares de integridad académica y científica. El artículo 6.2 del Reglamento General de Estudiantes de la UPR (Certificación Núm. 13, 2009-2010, de la Junta de Síndicos) establece que "la deshonestidad académica incluye, pero no se limita a: acciones fraudulentas, la obtención de notas o grados académicos valiéndose de falsas o fraudulentas simulaciones, copiar total o parcialmente la labor académica de otra persona, plagiar total o parcialmente el trabajo de otra persona, copiar total o parcialmente las respuestas de otra persona a las preguntas de un examen, haciendo o consiguiendo que otro tome en su nombre cualquier prueba o examen oral o escrito, así como la ayuda o facilitación para que otra persona incurra en la referida conducta". Cualquiera de estas acciones estará sujeta a sanciones disciplinarias en conformidad con el procedimiento disciplinario establecido en el Reglamento General de Estudiantes de la UPR vigente.