

## **PHZ 5156C, Computational Physics I (Spring 2025)**

**Instructor:** Dr. Inna Ponomareva; Office: ISA 5103; E-mail: iponomar@usf.edu; telephone: 974-7286

Prerequisites: Quantum Mechanics, Statistical Mechanics, Solid State at the graduate level or advanced undergraduate level. Check with Instructor to be sure.

Text: Computational Physics by J.M. Thijssen, second edition (available online through USF library, perhaps with some restrictions)

### Recommended books:

- A student's guide to PYTHON for physical modeling by J.M. Kinder and Philip Nelson, or any other introductory PYTHON book for those who do not have experience with PYTHON.
- Fortran by Samuel L. Marateck (available online through USF library, perhaps with some restrictions)
- Hack Your Brain: Secrets of an Elite Manhattan Tutor, by Elie Venezky and Patrycja Slawuta
- The Little Book of Talent: 52 Tips for Improving Your Skills, by Daniel Coyle
- Make It Stick: The Science of Successful Learning, by Peter C. Brown, Henry L. Roediger III, Mark A. McDaniel

Other resources: Computer with internet connection to perform homework.

Class: TR 9:30am-10:45am ISA 4010

Office Hours: W 8:30-9:30am, F 8:30-9:30 am and by appointment.

### **Course Outline and Objectives**

The course introduces students to computational physics and will cover the following topics: Linux, High Performance computing, script writing, programming with compiled and interpreted languages (Fortran and Python), Molecular Dynamics, Monte Carlo, Genetic Algorithm, Quantum Mechanical simulation techniques (variational method for Schrodinger equation, Hartree-Fock, Density Functional Theory, Schrodinger equation in periodic solids). Students will learn programming and will program all the aforementioned techniques. All work must be independently completed by each student, no group assignments.

<b>Course Grading Breakout</b>	Homework Problems	90 %
	Final	10 %

The GPA-inspired scale will be used to assign final letter grade for the course:

3.7 – 4.0 A	1.7 – 1.9 C
3.3 – 3.6 A-	1.3 – 1.6 C-
3.0 – 3.2 B+	1.0 – 1.2 D+
2.7 – 2.9 B	0.7 – 0.9 D
2.3 – 2.6 B-	0.3 – 0.6 D-
2.0 – 2.2 C+	0.0 – 0.2 F

## Tentative Schedule and Examination Dates

Week Beginning	Topics (Chapters in Text)
Jan 12	Linux/Unix operating systems; Shell programming, script writing
Jan 19	Coding with Fortran and Python.
Jan 26	
Feb 2	Molecular Dynamics (8)
Feb 9	
Feb 16	Monte Carlo simulations, equilibrium stat mech (7, 10)
Feb 23	
Mar 2	Optimization problem, genetic algorithm
Mar 9	Variational Method for the Schrodinger equation (3)
Mar 16	Spring Break
Mar 23	The Hartree-Fock method (4)
Mar 30	
Apr 6	Density Functional Theory (5)
Apr 13	
Apr 20	Solving Schrodinger equation in periodic solids (6)
Apr 27	
May 4	FINAL May 7 <sup>th</sup> , 7:30-9:30 am (tentative)

### NOTES

Students who anticipate being absent from exams due to a major religious observance must provide notice of the date(s) and event(s) to the instructor, in writing, by the second class meeting. Notes and Tapes are not permitted for purposes of sale.

Any student with a disability is encouraged to meet with me privately during the first week of class to discuss accommodations. Each student must bring a current Memorandum of Accommodations from the Office of Student Disability Services (974-4309, SVC1133) which is prerequisite for receiving accommodations. Accommodated examinations through the Office of Student Disability Services require at least two weeks notice.

USF has a set of central policies related to student recording class sessions, academic integrity and grievances, student accessibility services, academic disruption, religious observances, academic continuity, food insecurity, and sexual harassment that apply to all courses at USF. Be sure to review these online: [usf.edu/provost/faculty-success/resources-policies-forms/core-syllabus-policy-statements.aspx](https://usf.edu/provost/faculty-success/resources-policies-forms/core-syllabus-policy-statements.aspx)

### COVID NOTE

If class is to be moved on-line due to COVID we will continue meeting during the regular class times via zoom or other software. Webcamera, microphone, computer and internet are required for that. For examinations we will use on-line proctoring (honorlock).