PHY380: Introduction to Computational Physics

Spring 2024

Course Time and Location: TR 10:45-12:00 Lewis Lab 512

Instructor: David Rutkowski
Lewis Lab 416 | dmr518@lehigh.edu

Aim

The course will provide an introduction to computational modeling as an important tool in the study of physical, chemical and biological processes.

Textbook

H. Gould, J. Tobochnik, and W. Christian, "Computer Simulation Methods, Applications to Physical Systems" third edition. The book is freely available:
http://www.compadre.org/OSP/document/ServeFile.cfm?ID=7375&DocID=527

Course Format

Lecture Format: In person on computer and chalkboard.

Programming Language: One of the aims of the course is to develop modeling skills using a general-purpose programming language (such as Java, C, python, Fortran) and to introduce object oriented programming (OOP) concepts which are broadly applicable regardless of specific programming language. This course will be based on Java in order to use and take advantage of the framework developed by the Open Source Physics project (http://www.compadre.org/osp/index.cfm). Prior knowledge of Java is not required, but prior exposure to programming is expected.

Discussion and Individual meetings

We will use slack to facilitate discussion in groups and individually through messaging. Please use slack for comments or questions (instead of email), preferably through a channel accessible to the whole class. I will try to answer any questions, within a reasonable time frame, but anyone is welcomed to chime in.

I will be available for individual meetings (through zoom or in person), which can be arranged by sending me a direct message in slack.

Course Outline

Weeks 1 and 2. Introduction to Java and Open Source Physics (OSP). Chapters 1 and 2.
Week 3. Simulating Particle Motion. Chapter 3.
Week 4. Oscillatory Systems. Chapter 4.
Week 5. Few-Body Problems: The Motion of the Planets. Chapter 5.
Week 6. The Chaotic Motion of Dynamical Systems. Chapter 6.
Week 7. Random Walks and Chemical Reactions. Chapter 7.
Week 8. Molecular Dynamics Simulations of Many Particle Systems. Chapter 8.
Week 9. Normal Modes and Waves. Chapter 9.
Week 10. Electrodynamics. Chapter 10.
Week 11. Monte Carlo Simulation of Thermal Systems. Chapter 15.
Weeks 12 and 13. Quantum Systems. Chapter 16.
Week 14. Selected topic:

1. Python and Machine Learning
2. Running jobs on Sol and supercomputer clusters
3. Alternate computational topic

Initial Competences

• Basic programming skills.
• Knowledge of multivariable calculus, linear algebra and probability theory.
• Knowledge of Introductory/General Physics. Prior exposure to undergraduate-level classical mechanics, thermodynamics, electrostatics and introductory quantum mechanics.

Final Competences

• Ability to use a general-purpose programming language to develop and compile computer simulations.
• Understand concepts of numerical methods covered in class related to accuracy, speed, stability and conservation. This includes methods of integration of differential equations and random number generation.
• Use numerical methods to develop accurate simple simulations of physical, chemical or biological systems and compare to analytical approaches.
• Ability to identify the appropriate numerical approach depending on the system to be studied with simulations.
• Design and write code from scratch, making use of existing libraries. Communicate and summarize the method and results in both written and presentation format.

Grading

The course grade will be based on:
1. Homework (30%). No late homework submissions will be accepted. While you are encouraged to discuss assignments with other students in order to improve your understanding, you are nevertheless not allowed to share code. The submitted homework must reflect your own work.
2. Exams and Quizzes (25%).
3. Computational course project (45%). The topic of the project will be close to each student's interests and will be decided after discussion with the instructor.
4. A passing grade requires no more than three unjustified absences. This is a special requirement for this course since it's hard to catch up otherwise.

Office Hours

TR 12:00-1:00 Lewis Lab 416 (Tentative)

Accommodations for Students with Disabilities: Lehigh University is committed to maintaining an equitable and inclusive community and welcomes students with disabilities into all of the University's educational programs. In order to receive consideration for reasonable accommodations, a student with a disability must contact Disability Support Services (DSS), provide documentation, and participate in an interactive review process. If the documentation supports a request for reasonable accommodations, DSS will provide students with a Letter of Accommodations. Students who are approved for accommodations at Lehigh should share this letter and discuss their accommodations and learning needs with instructors as early in the semester as possible. For more information or to request services, please contact Disability Support Services in person in Williams Hall, Suite 301, via phone at 610-758-4152, via email at indss@lehigh.edu, or online at https://studentaffairs.lehigh.edu/disabilities.

The Principles of Our Equitable Community: Lehigh University endorses The Principles of Our Equitable Community:
http://www.lehigh.edu/ inprv/initiatives/PrinciplesEquity_Sheet_v2_032212.pdf. We expect each member of this class to acknowledge and practice these Principles. Respect for each other and for differing viewpoints is a vital component of the learning environment inside and outside the classroom.