

# PHY380: Introduction to Computational Physics

Spring 2017

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Time and Location: MF 11:10-13:00 Rauch 50

## 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

The course will be based on the Java programming language in order to use and take advantage of the tools developed by the Open Source Physics project (<http://www.compadre.org/osp/index.cfm>). Prior knowledge of Java is not required though prior exposure to programming is expected.

The course will be taught in a computer classroom, with each student having access to a computer. We will have two 2-hour sessions per week (Monday and Friday).

## Course Outline

**Weeks 1 and 2.** Introduction to Open Source Physics and Java. 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.** Fractals. Self-organized Critical Phenomena. Neural Networks. Chapters 12-14.

## 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 Java and Open Source Physics 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

Upon satisfactory attendance, the course grade will be based on:

**1. Homework (25%).** 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 and the submitted homework must reflect your own work.

**2. Exams and Quizzes (25%).**

**3. Computational course project (50%).** The topic of the project will be close to each student's interests and will be decided after discussion with the instructor.

**Note:** The use of computers during class time for activities unrelated to the course (facebook etc) is not allowed. This is disruptive to the course and students who fail to follow this guideline will be requested to withdraw from the class formally through a Section 3.

## Office Hours

TBA

Accommodations for Students with Disabilities: If you have a disability for which you are or may be requesting accommodations, please contact both your instructor and the Office of Academic Support Services, University Center C212 (610-758-4152) as early as possible in the semester. You must have documentation from the Academic Support Services office before accommodations can be granted.

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](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.