

Course Syllabus

PHZ 5155C Physical Modeling and Simulation

Fall 2020

Lectures

Lectures will take place via zoom every Tuesday and Thursday from September 1 through December 8 **except** November 26 (Thanksgiving Day). Classes will be held periods 5-6 (11:45 a.m.-1:40 p.m.) on Tuesdays and period 5 (11:45 a.m.-12:35 p.m.) on Thursdays.

Instructor

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Office Hours: Thursday 12:35 p.m.–1:35 p.m.

Course Overview

PHZ 5155C is an introduction to modeling and simulation in physics. Basic numerical methods used in computational physics are introduced. Topics covered including numerical interpolation, derivatives, integration; solutions to linear and nonlinear differential equations; linear algebra; Monte Carlo method; basics of classical molecular dynamics; and other topics in computational physics.

Textbook

The recommended textbook for this course is Computational Physics by Mark Newman, 2012. However, this is more of a reference as I will use my own notes and cover topics somewhat differently. In other words, you don't have to buy it. In addition, the following books can be very useful for this course and as references for future use:

- William H. Press, Saul A. Teukolsky, William T. Vetterling, Brian P. Flannery "Numerical Recipes 3rd Edition: The Art of Scientific Computing", 3rd edition, Cambridge University Press 2007. Then 2nd edition of this book is available for free online:

<http://apps.nrbook.com/c/index.html>

- David P. Landau, Kurt Binder "A Guide to Monte Carlo Simulations in Statistical Physics", 3rd edition, Cambridge University Press 2009.

- Michael T. Heath "Scientific Computing", 2nd edition, McGraw-Hill 2002. The content of this

book is available for free online as a course presentation:

<http://web.engr.illinois.edu/~heath/scicomp/notes/>

- Tao Pang "An Introduction to Computational Physics", 2nd edition, Cambridge University Press 2010.

- D. C. Rapaport "The Art of Molecular Dynamics Simulation", 2nd edition, Cambridge University Press 2004.

- R. M. Martin, "Electronic Structure", Cambridge University Press 2004.

HPC Account

To access the high-performance computing servers we will use during the course to run calculations, you must apply for a UF HPC account. Every UF student can apply for access to the HPC servers. Visit the website www.hpc.ufl.edu, click the 'Help Menu', and choose 'Request Account' from the dropdown menu. Fill in the required information and wait for approval. Once approved, you can access HPC by typing the following command in your terminal window:

```
ssh -Y username@gator.hpc.ufl.edu
```

The `-Y` is crucial because it allows graphics to be displayed from programs being run in the terminal window. If successful, you will be asked to enter your password and then be taken to your home directory. We will be compiling programs and running them on the HPC servers throughout the semester.

Homework

There will be seven homework sets, roughly every one to two weeks. All assignments will be distributed on the course website under "Files" in a subfolder "Homeworks". They must be turned in electronically on canvas before the start of the class on the day they are due. No credit will be given for late homework without exception.

You can use fortran, C, C++ or python for coding. You can also download the codes provided in the class as your starting point and make your own modifications. However, you may not copy codes from other students, even if you make further modifications. You can download codes from the web and use them as your starting point, but in that case you must have the license to use and distribute the codes (GPL is preferred), and you must state the source (where you got it) of the codes.

Exams

There will not be exams in this course.

Grades and grade points

The final grade will be calculated 100% from the sum of all homework grades. For information on current UF policies for assigning grade points, see <https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx>

Attendance requirement

Requirements for class attendance and make-up exams, assignments, and other work in this course are consistent with university policies that can be found at: <https://catalog.ufl.edu/ugrad/current/regulations/info/attendance.aspx>.

Academic honesty

UF students are bound by The Honor Pledge which states, "We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honor and integrity by abiding by the Honor Code. On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied: "On my honor, I have neither given nor received unauthorized aid in doing this assignment." The Honor Code (sccr.dso.ufl.edu/process/student-conduct-code/) specifies a number of behaviors that are in violation of this code and the possible sanctions. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor or TAs in this class.

Accommodation for Student with Disabilities: Students with disabilities who experience learning barriers and would like to request academic accommodations should connect with the disability Resource Center by visiting <https://disability.ufl.edu/students/get-started/>. This class supports the needs of different learners; it is important for students to share their accommodation letter with their instructor and discuss their access needs as early as possible in the semester.

Statement Regarding Evaluations: Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available from [the Gatorevals websiteLinks to an external site.](#). Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals, or via [the evaluation system.Links to an external site.](#) Summaries of course evaluation results are available to students at the [public results websiteLinks to an external site.](#)

Statement Regarding Course Recording: Our class sessions may be audio visually recorded for students in the class to refer back to and for use of enrolled students who are unable to attend live. Students who participate with their camera engaged or utilize a profile image are agreeing to have their video or image recorded. If you are unwilling to consent to have your profile or video image recorded, keep your camera off and do not use a profile image. Likewise, students who un-mute during class and participate verbally are agreeing to have their voices recorded. If

you are unwilling to consent to have your voice recorded during class, you will need to keep your mute button activated and communicate exclusively using the "chat" feature, which allows students to type questions and comments live. The chat will not be recorded or shared. As in all courses, unauthorized recording and unauthorized sharing of recorded materials is prohibited.