4600/5700. Computational Physics.

Instructor and office hours

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Office hours by appointment.

Schedule

This course takes place 100% remotely. We will have synchronous video conferences using Zoom at the allotted time (Tu-Th 9:30-10:50). Other than that, your interaction with me and with your fellow students will take place in Canvas. There are 14 weeks of content that you will move through. I will open up a new module almost every week.

Textbook (optional)

Rubin H. Landau, Manuel J. Paez, Cristian C. Bordeianu
Computational Physics: Problem Solving with Python
Wiley-VCH

Outline

This corse presents computational physics (CP) as a subfield of computational science. This implies that CP is a multidisciplinary subject that combines aspects of physics, applied mathematics and computer science (CS), with the aim of solving realistic and ever-changing physics problems. Other computational sciences replace physics with their discipline, such as biology, chemistry, engineering, and so on. Although related, computational science is *not* part of computer science. CS studies computing for its own intrinsic interest and develops the hardware and software tools that computational scientists use. Likewise, applied mathematics develops and studies the algorithms that computational scientists use. As much as we too find math and CS interesting for their own sakes, our focus will be on helping the student do better physics for which you need to understand the CS and math well enough to solve your problems correctly, but not to become an expert programmer.

Course Objectives

Upon successful completion of this course, you will be able to:

1. learn advanced python programming structures and fundamentals of modular programing etc.
2. given a physical problem, design the algorithm that will allow you to get results of computational experiments - develop your *computational scientific thinking*.
3. learn how to interpret the results of computational experiments in the context of physical and numerical approximations.
4. learn how to use computation of a meaningful interpretation of experimental or theoretical data structures.
5. learn the most efficient visualization techniques for the problem at hand.

Prerequisites

There are no required prerequisites for this course. However, in order to be successful in this course you will need to:

- have a basic computer literacy, including understanding of editors, shells, and installation of computing environments (installation of anaconda python is required)
- understand the basic logic of python programming structures, such as variables, iterators, logic statements etc.
- have the ability of designing algorithms for representative physics problems

Syllabus

Module 1. Review of python programming
Module 2. Newton-Raphson and multidimensional searching: static equilibrium
Module 3. Numerical derivatives and introduction to matrix computing (linear algebra)
Module 4. Static equilibrium as a linear algebra problem
Module 5. Quantum eigenvalues in arbitrary potentials
Module 6. Introduction to Fourier transform
Module 7. Fourier transform and noise filtering
Module 8. Fourier transform and digital signal processing (DSP)
Module 9. Thermodynamics simulations: Ising model and Monte-Carlo
Module 10. Thermodynamics simulations: Molecular Dynamics

Other subjects can be discussed upon completion of the required modules. For 5700 (graduate): projects based on current research activities are encouraged.

Grading

Grading will be based on the successful completion of the modules in the allotted time. Students will return their assignments as jupyter notebooks through Canvas.

The University of North Texas makes reasonable academic accommodation for students with disabilities. Students seeking reasonable accommodation must first register with the Office of Disability Accommodation (ODA) to verify their eligibility. If a disability is verified, the ODA will provide you with a reasonable accommodation letter to be delivered to faculty to begin a private discussion regarding your specific needs in a course. You may request reasonable accommodations at any time, however, ODA notices of reasonable accommodation should be provided as early as possible in the semester to avoid any delay in implementation. Note that students must obtain a new letter of reasonable accommodation for every semester and must meet with each faculty member prior to implementation in each class. Students are strongly encouraged to deliver letters of reasonable accommodation during faculty office hours or by appointment. Faculty members have the authority to ask students to discuss such letters during their designated office hours to protect the privacy of the student. For additional information see the Office of Disability Accommodation website at http://www.unt.edu/oda. You may also contact them by phone at 940.565.4323.

UNT's policy on Academic Dishonesty can be found at:
http://www.vpaa.unt.edu/academic-integrity.htm

Drop information is available in the schedule of classes at:
http://registrar.unt.edu/registration/schedule-of-classes

The Student Perceptions of Teaching (SPOT) is a requirement for all organized classes at UNT. This short survey will be made available to you on-line at the end of the semester and will provide you with an opportunity to provide feedback to your course instructor. SPOT is considered to be an important part of your participation in this class. In addition to SPOT, there will be a brief in-class course survey during the last two weeks of the semester.

Near the end of the Fall 2017 semester you will receive an email on from "UNT SPOT Course Evaluations via *IASystem* Notification" (no-reply@iasystem.org) with the survey link. Please look for the email in your UNT email inbox. Simply click on the link and complete your survey.

After logging in to the my.unt.edu portal, students can access the SPOT survey site by clicking on the SPOT icon. A list of their currently enrolled courses will appear. Students complete each course evaluation independently. During the long terms, the SPOT is open for students to complete two weeks prior to final exams. During the Fall term, the SPOT is open for students to complete six days preceding their final exam. See https://spot.unt.edu/content/fall-2017-8w1-calendar for specific dates and deadlines.