Physics 129AL: Fall 2023 (40709)
Version: September 6, 2023
Location: Broida Hall, 5223
Lecture: TR, 11:00AM-12:15PM
Instructor: Zihang Wang (zihangwang AT ucsb.edu)
Office: Broida 6304

Introduction to Scientific Computation

SYLLABUS

This course is a **physics orientated** survey of basic concepts in modern computation, and the following outline is subject to change:

- **Foundations of modern computation**, hardware and software, input/output (I/O), UNIX operating system (os), UNIX shell and file management, bash script, version control, network, data acquisition (DAQ)*.

- **An introduction to Python**, basic programming, data structures, read/write, functions, scoping*, objects, error handling*, debugging*, pipe*, parallel computing.

- **Important Python packages**, os, Numpy, Matplotlib, Scipy*.

- **Common statistical methods in physics**, random process, probability density function (PDF), central limit theorem, Bernoulli process, binomial process, Poisson process, Lorentz (Cauchy) distribution.

- **Common computation techniques in physics**, discrete Fourier transform, numerical integration and differentiation, implicit and explicit iterative methods for differential equations, gradient descent, stochastic sampling, Monte Carlo, Markov chain, PID control, machine learning, and deep learning.

- **Applications in physics**, Electrostatics, Diffusion, Brownian motion, driven system, hydrodynamics, phase transitions, molecular dynamics, *ab initio* approaches to electronic structure, quantum state (Qubit) evolution, numerical renormalization group.

This course is **not** a theoretical physics course, but rather a survey of modern computation in physics. Therefore, I will provide **all** necessary physics background/concepts to you along the way. However, students are expected to have basic knowledge in classical mechanics, quantum mechanics, and statistical mechanics. By the end of this course, you will be asked to complete an independent project, choosing from selected physics topics.

EQUIPMENT REQUIREMENTS

Following the physics department guidelines, students are recommended to purchase a specific raspberry pi 4 kit, but in this course, you are not required to have one. For the first part of the course, students are expected to have **a Linux kernel** installed to preform necessary tasks. In the remaining of the course, we will use **Jupyter notebook**, e.g. https://www.anaconda.com/download. We will discuss the requirements in details during the first lecture.

TEXTBOOKS

The two textbooks are optional for your own reference,

- The Linux Command Line, Fourth Internet Edition William E. Shotts, Jr.
- A Student's Guide to Python for Physical Modeling: Updated Edition J.M Kinder and P. Nelson

PROBLEMS SETS AND PROJECTS

There will be approximately **six (6) problem sets** and **one (1) final project**. Late homework will not be accepted except at the discretion of the instructor. Most of the problem sets will be posted in the *.ipynb* format, and your lowest problem set score will be dropped. Please check instructor announcements frequently to avoid delays.

FINAL EXAM

One pen and paper final exam will be given in the scheduled time, **Wednesday, December 13, 2023 12:00 PM - 3:00 PM**. You are allow to bring a single-page cheat sheet (any size), but it must be hand-written.

LECTURES, DISCUSSION SECTIONS, AND OFFICE HOURS

Lectures are on Tuesday and Thursday from 11:00AM to 12:15 PM pacific time in Broida 5223. The instructor will introduce related backgrounds and concepts that are closely related to the problem sets. There are two **discussion sections**,

- Monday and Wednesday from 2:00PM-3:50PM, Broida 5223 (40717)
- Tuesday and Thursday from 1:00PM-2:50PM, Broida 5223 (40725)

and teaching assistants (TAs) will answer any course related concerns, including backgrounds, concepts, clarifications, etc. **Office hours** for both the instructor, Zihang Wang (zihangwang AT ucsb.edu) and TAs will be announced in the first lecture, or by appointments. The instructor is available for pre-scheduled meetings, as well as drop-in meetings, (Office location: Broida 6304).

GRADING

A letter grade will be assigned based on the following weighted average:

- **Five Problems Sets** (after dropping the lowest score): 50%
- **Final Project**: 30%
- **Final Exam**: 20%

COURSE POLICY

Requests for extensions will be considered on an individual basis. Any code and related work **must** be written by the student who submits the work. You are encouraged to work with other students and explore generative AI models while working on problems, e.g. GPT, Co-pilot... However, you must type/write/explain the work in you own words.

DSP ACCOMMODATIONS

Reasonable accommodations will be granted to students with disabilities, and please inform the instructor via email by the end of the first week of instruction.

COURSE CONTENT

The weekly schedule, subject to change, is given below.

WEEK 1

1. Introduction to the course and software installation.
2. Basics on Linux shell and file management, **Problem set 1**

WEEK 2

1. Bash script and version control
2. Network protocols, **Problem set 2**

WEEK 3

1. Introduction to Python
2. Introduction to Python packages, **Problem set 1 due, and Problem set 3**

WEEK 4

1. Introduction to statistical methods in physics
2. Statistical methods in physics, continue, **Problem set 2 due and Problem set 4**

WEEK 5

1. Numerical integration and differentiation, implicit and explicit iterative methods for solving differential equations
2. Gradient descent, stochastic sampling, Monte Carlo, Markov chain, PID control, **Problem set 3 due and Problem set 5**

WEEK 6

1. Discrete Fourier transform, machine learning, and deep learning
2. Electrostatics: Laplace's equation and Poisson's equation, **Problem set 4 due and Problem set 6**

WEEK 7

1. Simple diffusion
2. Driven systems, **Problem set 5 due and Final project**

WEEK 8

1. Brownian motion
2. Phase transition, **Problem set 6 due**

WEEK 9

1. Density functional theory
2. Quantum state (Qubit) evolution

WEEK 10

1. Numerical renormalization group
2. Final Review, **Final project due**

WEEK 11

Final Exam: Wednesday, December 13, 2023 12:00 PM - 3:00 PM
