Physics 650, Section 75 – Spring Semester 2018 Research Methods in Physics & Astronomy

Instructors

This course is being taught sequentially this semester by three faculty members of the Department of Physics & Astronomy –

Professor Chakram S. Jayanthi Natural Science Building 102 Email: chakram.jayanthi@louisville.edu Telephone: 502.852.0851 Office Hours: 1:00 - 2:15 Mondays, or by appointment

Assistant Professor Swagato Banerjee Natural Science Building 210 Email: swagato.banerjee@louisville.edu Telephone: 502.852.0915 Office Hours: 1:00 - 2:15 Mondays, or by appointment

John Kielkopf Department of Physics and Astronomy Natural Science Building LL01 University Email: kielkopf@louisville.edu Google Mail: jkielkopf@gmail.com Telephone: 502.852.5990 Video Conference: Zoom Meeting 5116430632 I am available Tuesday evenings after class. For prompt email response or if you need help with a computing assignment, use my gmail account jkielkopf@gmail.com. We can share

desktops with either Zoom or Hangouts if needed

Where and When

The class will meet every Tuesday and Thursday from 5:30 to 6:45 PM. The first part, led by Professor Jayanthi, will have lecture sessions usually held in NS 104 (Adams room) and interactive computer lab sessions in NS 134 (the TEAL classroom facility) and NS 132 (the Linux Computing Cluster facility). The second part led by Professor Banerjee will meet in the TEAL classroom. After Spring Break the last part with Professor Kielkopf will meet in the conference classroom NS 312. Topics and dates are provided below.

Objectives

This course is a survey of research methodologies that in this term are drawn primarily from computing and data analysis techniques, and are broadly applicable for graduate students who are engaged in doctoral level research. With the objective of providing useful tools and a perspective on how advanced scientific research is conducted, we will cover three topics this semester:

- 1. Numerical methods (Jayanthi)
- 2. ROOT, a language for data mining and machine learning (Banerjee)
- 3. Essentials of Python, with Javascript and data visualization (Kielkopf)

This is a required course for students in the doctoral program in Physics & Astronomy.

Requirements

Students should be enrolled in the graduate program in Physics & Astronomy or have comparable experience.

You are expected to

- 1. Attend and participate in all classes
- 2. Study the in-class and on-line material for the topics
- 3. Respond in a timely way to homework assignments

Blackboard and other websites

The gateway for this course is the University's Blackboard system,

http://blackboard.louisville.edu/

which offers access to announcements and to grades. Your University *User ID* and *Password* are required to log into Blackboard.

An instructional site for the section on Python with other useful links is

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http://prancer.physics.louisville.edu/classes/650/
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There may be other websites used in this class to support the topics covered, and they will be linked on Blackboard, the class site above, and described in class meetings.

Textbooks, software, and computer access

There are no required textbooks. For the last section, on Python and Javascript, the book "Data Visualization with Python & Javascript" by Kyran Dale is recommended. There will be material offered in class and on the websites for all sections.

Students in this class will use the Mac OSX systems in the TEAL classroom (NS 134) and the Linux computing cluster (hpclab2.physics.louisville.edu) in the adjacent room (NS 132). Access to to your own desktop, laptop or tablet will be useful since that will provide a remote connection to the Linux server, and often a way to install some of the software we will use in class for your own applications later. The last part of the course, emphasizing Python and Javascript, will require your use of your own computer but any operating system (OSX, Windows, Linux, and Chrome) will work.

Topic 1 – Numerical methods – Jayanthi

Dr. Jayanthi's lectures will give an overview of numerical methods and algorithms that are commonly used in solving physics problems using computers. Her lectures will review essential Linux commands, Programming using Fortran 90, numerical methods for integration, differentiation and root finding; finite difference and relaxation methods for solving partial differential equations; solving eigenvalue problems, Monte Carlo (stochastic simulation) and Molecular Dynamics (deterministic simulations). These algorithms will be illustrated through simple case studies.

Samples of in-class projects to be conducted by students are listed below:

- 1. Numerical Integration Trapezoidal and Simpson Rules, Monte Carlo integration.
- 2. Numerical Solutions of Differential Equations: Euler, Verlet, and Runge-Kutta algorithms

Case Study: One-Dimensional Simple Harmonic Oscillator

- 3. Root Finding: Newton Raphson and Bisection methods.
- 4. Partial Differential Equations: Relaxation Method Case Study: Solving Laplace Equation with boundary conditions
- 5. Monte Carlo Simulations– Metropolis Algorithm Case Study: Ising Model
- 6. Numerov Algorithm combined with the Shooting and Matching Method for solving boundary value PDE problems

Case Study- Bound states of a particle in a box

7. Eigenvalues, Eigenfunctions, and Green's Functions

Case Study: The vibrational Dynamics of a Vicsek fractal

8. Elements of Molecular Dynamics Simulation

Final Requirement: Students will be required to complete an independent computational project of their choice and give an oral presentation. Students must submit reports of all in-class projects to receive a passing grade in this section.

Reference Materials

- 1. Linux for Dummies (Sixth Edition).
- 2. Fortran 90 for Engineers and Scientists by Larry Nyhoff and Sanford Leestma
- 3. Computational Physics by Rubin H. Landau and Manuel Paez
- 4. Computational Physics by N.J. Giordano

Topic 2 – ROOT, a language for data mining – Banerjee

The second topic of the course will be an introduction to ROOT and its use in data analysis. ROOT is a modular scientific software framework, available for free usage from https://root.cern.ch. It provides all the functionalities needed to deal with big data processing, statistical analysis, visualisation and storage. It is mainly written in C++ but integrated with other languages such as Python and R. Makefiles provide powerful methods for standalone compilation using ROOT libraries in UNIX-like platforms. We will learn graphical methods to visualize data with multi-variate atributes, and machine learning techniques for signal over background separation. The principle of maximum likelihood ratio can be demonstrated as a basis of all modern artificial neural network classifiers. It is imperative that students demonstrate that their projects actually work during presentations in class during this topical section.

Topic 3 – Essential Python, Javascript, and WebGL – Kielkopf

In this topic we will introduce you to writing your own programs using Python with examples drawn from astronomy, astrophysics, and optics. We will discuss the merits (and pitfalls) of programming in contrast to using commercial or community-based programs, and compare commonly used languages and tools. Python was chosen because it is free, flexible, and now widely used in physics, astronomy, space science, and engineering. Prior experience with programming is not required. We will use the time available to help you develop core skills that you can turn to in your own research. Along with Python, we will also introduce Javascript, the browser-based programming language that is extremely powerful for graphic user applications and for website development. Javascript provides an introduction to graphical language programming, and to graphical processing unit (GPU) computing. Open source Python and Javascript libraries add to a high quality interactive tool chain for understanding and analyzing scientific data.

Each student will have an individual project in Python or Javascript relevant to their research interests that they develop during this topical period and present to the class during its last week.

Grades

This is a Pass/Fail course and it will be graded as an average of the 3 grades for each topic, assigned by the faculty teaching that topic. All topics include two components: incluss participation on projects and activities with required attendance, and a presentation of a project for the instructor and the class at the end of the topic. Those parts will be weighted equally in determining the grade for that component, and consequently attendance is mandatory for passing this class.

Caveats

We reserve the right to make changes in the syllabus when necessary to meet learning objectives, or when there is a technical or software issue that requires a change in content or methodology. Any changes will be announced in class, by email, and posted in the current on-line syllabus and schedule.

Numerical methods (Jayanthi)

9 January and 11 January Basic Linux commands and elements of programming

- 16 January and 18 January Numerical Integration/ Numerical Differentiation
- 23 January and 24 January Root Finding Methods
- 30 January and 1 February Boundary Value Problems/ Monte Carlo
- 6 February and 8 February Student Presentations

ROOT and data mining (Banerjee)

13 February and 15 February ROOT: Introduction, Functions and Histograms

20 February and 21 February Histograms, Graphs and Ntuples

- 27 February and 1 March Standalone Makefiles and Macros
- 6 March and 8 March Multi-variate discriminators and Student's Presentations
- 13 March and 15 March Spring break

Python and Javascript Programming (Kielkopf)

- 20 March and 22 March Getting started with simple Python. Data types, lists, flow control, and functions
- 27 March to 29 March Scientific computing with Numpy and Scipy
- **3 April to 5 April** Managing data with Python using Numpy, Pandas, and even spreadsheets
- 10 April to 13 April A simple server with Python. Interfacing Python to the web with Javascript and D3.js
- 17 April to 19 April Presentations of your work for this topic.

Title IX/Clery Act Notification

Sexual misconduct (including sexual harassment, sexual assault, and any other non-consensual behavior of a sexual nature) and sex discrimination violate University policies. Students experiencing such behavior may obtain confidential support from the PEACC Program (502.852.2663), Counseling Center (502.852.6585), and Campus Health Services (502.852.6479). To report sexual misconduct or sex discrimination, contact the Dean of Students (502-852-5787) or University of Louisville Police (502.852.6111).

Disclosure to University faculty or instructors of sexual misconduct, domestic violence, dating violence, or sex discrimination occurring on campus, in a University-sponsored program, or involving a campus visitor or University student or employee (whether current or former) is not confidential under Title IX. Faculty and instructors must forward such reports, including names and circumstances, to the University's Title IX officer.

For more information, see the Sexual Misconduct Resource Guide.