PHYS/CHEM 229A & PHYS100 Computational Methods

Mathematical, computational/numerical analyses in Physical Sciences using Mathematica

https://canvas.eee.uci.edu/courses/39928

Tues & Thurs 3:00-4:20 pm (Lecture MSTB-114)

Tues 2:00-2:50 pm (Lab session DBH-1425)

Office hour: Wed 11:30 am -12:30 pm (Zoom Meeting by appointment)

First/Last day of class: Sept 23rd Thurs / Dec 2nd Thurs

Final: Dec 7 Tues 4:00-6:00 pm or take-home

Recommended textbooks:

- MathematicaHandbook (Mathematica-based notebook by Peter Taborek)
  https://mathematica-handbook.com/
  Contents: http://www.mathematicahandbook.com/videos/TOCNarrow.html
  Click on get installer-> Download installer; run the installer in Mathematica using the transaction code (by purchase). Note that Mathematica is free for all UCI students (check OIT: KB0010917)
  - Python/Matlab e.g. Programming for Computations-Python/Matlab (you can try if you want; we use Mathematica in current class)
    Springer Open online: http://hplgit.github.io/prog4comp/
- "Mathematical Methods for Physicists" by Arfken and Weber
- "Mathematical Methods in the Physical Sciences" by Boas
- "Computational Methods for Physics" by Franklin
- ... You pick one and keep it working with you for constant usage

Course Contents & Schedules special topics for Lab session (subject to adjustments)

- Syllabus and Preliminaries week 0 or 9/23 Thurs
- Linear Algebra and Vector Analysis week 1-2 or 09/28-10/7;
  + Mathematica usage tutorial
  + Lagrange multipliers and constrained optimization
- Complex Variables (+ Simulation & Sampling Methods) week 3-4 or 10/12-21;
  + Fourier series, transforms, and expansions (cont.)
  + DiracDelta and other generalized functions
- Ordinary Differential Equations week 5-6 or 10/26-11/4;
  + Dimensional analysis + Asymptotic analysis
- Partial Differential Equations week 7-8 or 11/9-18 (no class on 11/11);
  + Perturbation theory + Calculus of Variations
- Probabilities and Statistics (+ Learning & Stochastic Methods) week 9-10 or 11/23-12/2 (no class 11/25) + Calculus of Variations (cont.)

- Case Studies Individual group presentation (Lab session week 4/8/10)
  Choose one topic below or discuss with me **your own proposal**, decide early

Circuits	Review of elementary circuits, impedance, LRC circuits, switches
Normal Modes	Animations of blocks on springs, density of states, linearization
Fresnel Equations	Reflection and refraction of a vector wave at an interface
Wave Guides	Electromagnetic waves confined by conductors and dielectrics
Thermodynamic Derivatives	Symbolic calculations of thermodynamic derivatives
Fluid Mechanics	Navier-Stokes equation, vector Laplacian, vorticity
Multipole Expansions	Far field solutions to Laplace equation using cartesian tensors and spherical harmonics
Numerical Integration	Accuracy, Precision, Monte Carlo integration
Digital Sampling	Digital scope simulator, aliasing, Nyquist critical frequency
N Body Simulation	Simulating a gas of hard spheres; animations
Quantum Square well	Bound states of a 1D potential well

Quantum Harmonic Oscillator	Solution of quantum oscillator problem using series and DSolve
Hydrogen Atom	Schrödinger equation for hydrogenic atom; 3D graphics
Statistical Learning Basics	*Contact me to discuss options*

Course policy and grading etc.

- Lab & Lecture on Tues (2 pm-4:30 pm)
  Lab: 2-2:50 pm Special topics first (~30 mins, with **Discussion and/or Quiz** see topics in course contents, Lab session score 1 point/session, see below); then we run **Q/A** & **peer-review homework grading** session (~ 20 mins; we may occasionally arrange Case study presentation in this session). There is a 10-min break in the end to lecture.
  Lecture: 3-4:20 pm Short Q/A: 4:20-4:30 pm
- Lecture on Thurs (3:00 pm-4:30 pm)
  Lecture: 3-4:20 pm Short Q/A: 4:20-4:30 pm

Note: Former course materials would be shared online prior to each week's courses, so it is possible to pre-view course contents in advance; current (updated) lecture notes will be made available online after each class

- Homework (HW) assignments, submission, and grading policies
  - 10 HW problem sets (week 0-9)
  - New assignment usually posted online Tues evening/Wed morning, due ~6 days by next Mon (11:59 pm)
  - You choose 3-5 problems to finish among those provided
  - Solutions posted online Tues morning (late submission after solution posted gets 30% scores you obtain; no further submission can be made after Tues hence no score)
  - We grade each other online in Tues lab second session (i.e., one grades another via Canvas peer-review grading system)
  - 10 points each set and a total of 100 points
  - Account for **50% of your final grades**

Note: We have **two participation scores optional** to replace two lowest HW scores (e.g.to make it up for accidental late/missing submission):
1) 10-point overall participation score (peer grading +4 point; class participation +2 point; midterm survey +2 point; final evaluation +2)
2) 10-point Lab/Discussion session score (1 point each session by signed sheet)

- Final Exam In class or take-home (to be decided)
  Account for **30% of your final grades**
- Case study group presentation You have option to do it in some Lab session, otherwise we arrange in the last day class; each individual group (e.g. 2 persons) chooses one topic (see Case studies above) as early as possible, and presents to the full class; account for **20% of your final grades**

Mathematica preliminaries → We start working on Sept 23rd (with HW1 due incoming Tues)
Mathematica Usage Tutorials in the MathematicaHandbook (it is useful & can be fun)

Intro to Mathematica 1&2	Basic syntax, intro to replacement rules and functions; Plotting, DEs, multi-line functions
Vectors & Integrals	Operations on vectors, multiple integrals, 3D graphics
Basic Numerical Functions	FindRoot, NSolve, LinearSolve, NIntegrate, etc.
Input & Output	Importing and Exporting spreadsheets, graphics, etc.
Plotting&Graphics Examples	Many examples of 2D and 3D graphics, animations, etc.

Mathematics preliminaries If you have not learned topics like linear algebra in college, pls prepare yourself on the basics before class.