PHYS 100/229A or CHEM 229A. Computational Methods

Mathematical and numerical analysis using Mathematica etc in physical sciences

https://canvas.eee.uci.edu/courses/30246

Tues & Thurs 3:00-4:20 pm (Lecture); Tues 2:00-2:50 pm (Lab session)

Office hour: Thurs 4:20-5:00 pm (right after the lecture)

First/Last day of class: Oct 1st Thurs / Dec 10th Thurs

Final: Dec 15 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 subject to adjustments + special topics for Lab session

- Syllabus and Preliminaries week 0 or Oct 1st Thurs
- Linear Algebra and Vector Analysis week 1-2 or Oct 6-15;
  + Mathematica usage tutorial
  + Lagrange multipliers and constrained optimization
- Complex Variables (+ Sampling Methods I) week 3-4 or Oct 20-29;
  + Fourier series, transforms, and expansions (cont.)
  + DiracDelta and other generalized functions
- Ordinary Differential Equations week 5-6 or Nov 3-Nov 12;
  + Dimensional analysis + Asymptotic analysis
- Partial Differential Equations week 7-8 or Nov 17-26 (no class on 11/26);
  + Perturbation theory + Calculus of Variations
- Probabilities and Statistics (+ Sampling Methods II) week 9-10 or Dec 1 & Dec 10
  + Calculus of Variations (cont.)
- Case Studies Group presentations (Lab session or week 4/8/10 in class)
  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

Course policy and grading etc.

- Lab & Lecture on Tues (2 pm-4:30 pm)

  Lab: 2-2:50 pm Special topics first (see p1 course contents; 30 mins); then we run **Q/A** and **peer-review homework grading** session together; occasionally, we can also arrange Case study presentation in this session. There is a 10-min break.

  Lecture: Tues 3-4:20 pm Via Zoom, we take two lecture sessions: 3-3:30 pm & 3:50-4:20 pm; in between is a focused **Discussion** session 3:30-3:50 pm. We leave a 10-min short Q/A session 4:20-4:30 pm.

- Lecture & Office Hour on Thurs (3:00 pm-5:00 pm)

  Lecture: 3-4:20 pm Via Zoom, we take two lecture sessions: 3-3:30 pm & 3:50-4:20 pm; in between is a focused **Discussion** session 3:30-3:50 pm.

  Office Hour: 4:20-5:00 pm We have 40-min individual communication time.

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

- Homework assignments, submission, and grading policies
  - 10 HW problem sets (week 0-9)
  - New assignment usually posted online on Tues, due 6 days on Mon
  - 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 on that)
  - 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: there is a proposed 10-point "participation score" (peer review grading +4; class participation +2; midterm survey +2; final evaluation +2), which can be used to replace one lowest HW score.

- 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, or we can arrange some in the class session in week 4/8/10
  2-3 persons form one group; each group chooses one topic (see page 1) as early as possible, and presents to the full class; account for **20% of your final grades**

Mathematica preliminaries → We start working on that week 0 or Oct 1st

Mathematica Usage Tutorials in the MathematicaHandbook (it can be fun)

Intro to Mathematica 1	Basic syntax, intro to replacement rules and functions
Intro to Mathematica 2	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. Using Wolfram curated data e.g. Financial Data
Plotting& Graphics Examples	Many examples of 2D and 3D graphics, animations, etc.

We leave HW1 on this after the first class, and check on that next Tues Lab (Oct 6th).

- *Wolfram Documentation/Website under Help menu of Mathematica*

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