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/
  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 pl 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 Mathematica Handbook (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.