PHYS/CHEM 229A & PHYS100  Computational Methods
Mathematical, computational/numerical analyses in Physical Sciences using Mathematica
https://canvas.eee.uci.edu/courses/57998
Tues & Thurs 12:30-1:50 pm (Lecture PSCB 240)
Tues 2:00-2:50 pm (Lab session DBH-1425)
Office hour: Thurs 2 pm -3 pm (Office RH 210K or Online via Zoom)
First/Last day of class: Sept 28th Thurs / Dec 7th Thurs
Final: Dec 15 Fri 10:30-12:30 pm (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 09/28 Thurs
- Linear Algebra and Vector Analysis  week 1-2 or 10/03-10/12;
  + Mathematica usage tutorial (Python version undergoing)
  + Lagrange multipliers and constrained optimization
- Complex Variables  week 3 or 10/17-19;
  + Fourier series, transforms, and expansions (cont.)
- Simulation & Sampling  week 4 or 10/24-26
  + DiracDelta and other generalized function
  Midterm Survey
- Ordinary Differential Equations (ODE)  week 5-6 or 10/31-11/9;
  + Dimensional analysis + Asymptotic analysis
- Partial Differential Equations (PDE)  week 7 or 11/14-16
  + Perturbation theory
- Probabilities and Statistics  week 8/9 or 11/21-28 (no class 11/23 thx giving)
  + Calculus of Variations + Calculus of Variations (cont.)
- Stochastic Methods  week 9/10 or 11/30-12/05
- Case study presentations  week 10 12/05-12/07 (Tues Lab + Thurs lecture)
- Case study topics (Individual project; 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.

- **Lecture + Lab on Tues (12:30 pm-2:50 pm)**
  
  **Lecture: 12:30-1:30 pm**  
  Special topics brief review first (~10 mins); the student-lead Discussion and Problem session (20 mins; see topics in course contents);  
  the Q/A & peer-review homework/grading session (20 mins); 1 point for lab participation, 3 points for leading the session, **10 points total or 10% of your final grades**

- **Lecture + office hour on Thurs (12:30 pm-2:50 pm)**
  
  **Lecture: 12:30-1:30 pm**  
  **Office hour: right after the lecture at 2-2:50 pm**

- **Lecture course participation** (1 point each lecture with in-class problem sheet submission; **20 points total or 10% of your final grades**)

- **Homework (HW) assignments, submission, and grading policies**
  
  - **8 HW problem sets** (week 0-3,5-8)
  - New assignment posted online Tues evening/Wed morning (except for week 0 on Thurs), due by next Mon (11:59 pm on Canvas)
  - You choose 3-5 problems to finish among those provided
  - Solutions posted online Tues morning (late submission after solution posted gets 30% scores; no further submission/score after Tues)
  - One grades another via Canvas peer-review grading system
  - 10 points each set (8 points problems + 2 points on peer grading)
  - **80 points total or 40% of your final grades**

  **Note:** one optional score to replace one lowest HW score (e.g. for accidental late/missing submission): 10-point total (midterm survey +4 point; final evaluation +6 point)

- **Final Exam**  
  take-home; **25% of your final grades**

- **Case study presentation**  
  mainly arranged in class the last week; one chooses one topic (see Case studies above) as early as possible, and presents ~15 mins to the full class for review; **account for 15% of your final grades**

**Mathematica (Python?) preliminaries**  
We start on Sept 28th (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**  
College linear algebra or prepare yourself before class

**Note:** Supporting Neurodiversity in the Classroom