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: 12:30-1:50 pm
  Lab: 2-2:50 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: 12:30-1:50 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