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

Mathematical and numerical analysis using Mathematica etc in physical sciences

https://canvas.eee.uci.edu/courses/19793

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 with you for constant usage

Course Contents & Schedules subject to adjustments; + special topics in Tues Lab

- Syllabus and Preliminaries week 0 or Sept 26
- Linear Algebra and Vector Analysis week 1-2 or Oct 1-10;
  + Fourier series and Transforms
- Complex Variables week 3-4 or Oct 15-24;
  + DiracDelta & Generalized functions
- Ordinary Differential Equations week 5-6 or Oct 29-Nov 7;
  + Lagrange Multipliers + Units and Dimensions
- Partial Differential Equations week 7-8 or Nov 12-21;
  + Calculus and Variations + Asymptotic Analysis
- Probabilities and Statistics week 9-10 or Nov 26 & Dec 3
  + Perturbation Theory
- Applications and Case Studies week 10 or Dec 5 group presentation
  Each group (2-3 persons self-organize) pls choose one below as 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.

- Lecture: Tues and Thurs 3-4:20 pm HH 105
  Pls come on time, class attendance >80% is expected
  See course contents and schedules on page 1

- Lab: Tues 2-2:50 pm DBH 1425 Yes we break & walk to the Lecture Room + special topics (see page 1 course contents; 30 mins)
  & we review and grade homework for each other (one-one, use peer-review grading system online or an automated tool; 20 mins)

- Homework assignments, submission, and grading policies
  - 10 HW problem sets (week 0-9)
  - New assignment posted online on Tues, due 5 days on Sun
  - You choose 5 problems to finish among those provided
  - Solutions posted online Mon (late submission recorded, get 30% scores you obtain on Tues, no submission before Tues Lab no score)
  - We grade each other online in Tues lab (i.e., one grades another or we use an automated tool)
  - 10 points each set (2 pts each problem) and a total of 100 points
  - account for 50% of your final grades

- Final Exam Dec 7-13
  Likely, we do take-home exam, e.g. you choose 5 or 6 problems among 10 to solve; account for 30% of your final grades

- Case study group presentation Dec 5 Thurs
  2-3 persons form one group; each group chooses one case study (see page 1) as early as possible to go through it, and presents on the last day of class; account for 20% of your final grades

Mathematica preliminaries → We start working on that week 0 or Sept 26, the first class and right after

- Mathematica Usage Tutorials in the MathematicaHandbook
  HW problem set 1, and we discuss immediately on next Tues Oct 1st Lab
- Wolfram Documentation/Website under Help menu of Mathematica
- ... You find your own resources

Mathematics preliminaries be alert if you don't know much about the things when you go through the above Mathematica Usage Tutorials; you can make it up though …

- "Mathematical Methods for Physicists" by Arfken and Weber, Chapter 1
  not that easy maybe: Infinite series, Series of Functions, Binomial Theorem, Mathematical Function, Operations on Series Expansions of Functions, Some important Series, Vectors, Complex Numbers and Functions, Derivatives and Extrema, Evaluation of Integrals, Dirac Delta Function;

  Chapter 2 on Determinants and Matrices, and Chapter 3 on Vector Analysis (for grads)

- … college mathbooks?