PHYS474: "Computational Physics"

- Description: This course provides an overview of some of the most widely used methods of computational physics, including numerical integration, numerical solutions of differential equations, molecular dynamics simulations, and Monte Carlo simulations. In addition to giving the students a basic working knowledge of these particular techniques, *the goal is to make them proficient in scientific computing and programming in general, so that they will be prepared to tackle also other computational problems that they may encounter in the future.* (3 credits).

- Prerequisites: ~~PHYS404 (Stat. Mech.)~~; and PHYS373 (Math. Methods II); and (PHYS165, CMSC106, or CMSC131). A working knowledge of Linear Algebra is *strongly* recommended. Matlab will be used throughout this course; you must be familiar with its basic use [or a scientific programming language such as C (and its variants), python, FORTRAN, etc]. I also strongly recommend first taking PHYS401 and PHYS411.

- Instructor: Prof. Ian Appelbaum, Physical Sciences Complex, Rm. 2154.

  Phone: x5-0890 / e-mail: appelbaum@physics.umd.edu

  Please arrange a meeting time via email to discuss grades or other personal situations including absences. I strongly encourage the use of asynchronous communications on course material via the ELMS discussion board.

- TA: Mr. Dedi Wang, John S. Toll Physics Building 0220.

  Phone: x5 5969 / e-mail: dwang97@umd.edu

- Course Web Site: There is no textbook for this course. All course materials, including this syllabus, homework assignments, solutions, lecture notes, etc. will be posted to UMD ELMS.

- Schedule: 3:00pm–4:15pm, Monday and Wednesday in JMP 1109.

- Homework: You will be assigned to implement the algorithms and obtain the results discussed in lectures. Submit your code and output including figures directly to the TA via email within 2 weeks of the corresponding lecture.

- Grading: Your course (letter) grade is determined – at the END of the semester – by your numerical scores on homeworks (80%) and one final exam (20%). Plus/minus grades will be avoided.

- Dropping the Course: The last day to drop the course is April 10.

- UMD course policy

Informal guide to topics covered in this course:

- Mechanics
  - Equations of motion: Verlet algorithm
  - Distributed systems: partial-differential equations, finite differences, and the Crank-Nicholson method, basis vectors and eigenproblems, boundary conditions
- E & M
  - Electrostatics: Laplace and Poisson equation
  - Dynamics: Wave propagation, resonance, transfer matrix method, diffraction and interference
- Statistical Mechanics
  - Random thermal motion: Metropolis-Hastings, Drift-diffusion
  - Phase transitions: Ising model of ferromagnetism
- Quantum Mechanics
  - Bound states: finite-differences and variational method, perturbation theory
  - Self-consistent Schrödinger-Poisson solution
  - scattering: transfer matrix, Green's functions and self-energy
  - periodic potentials and bandstructure

Also:
signal processing (FFT, polynomial interpolation, etc.), error analysis, computational complexity, root finding, Monte-Carlo, sparse matrix methods, Hopfield networks, quadrature . . .

If you choose to use a language other than Matlab or GNU Octave, you must be proficient with its implementation of random number generation and operations in linear algebra (including complex and sparse matrices): matrix multiplication, inversion, eigenvalues/vectors, etc. It is also helpful to have a FFT, and you will need to plot in 2- and 3-D.