PHYS 516: METHODS OF COMPUTATIONAL PHYSICS
Spring 2020 (class number: 50614R)

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Lecture: 9:00-9:50 am M W F, WPH 206

Office Hour: 4:00-4:50 pm F

Course Page: http://cacs.usc.edu/education/phys516.html

Textbooks: T. Pang, *An Introduction to Computational Physics, 2nd Ed.* (Cambridge Univ. Press, 2006)—sample C, Fortran 77, and Fortran 90 programs at www.physics.unlv.edu/~pang/cp.html

W. H. Press, B. P. Flannery, S. A. Teukolsky and W. T. Vetterling, *Numerical Recipes, 3rd Ed*. (Cambridge Univ. Press, 2007)—available online (C: www.nrbook.com/a/bookcpdf.php or Fortran: www.nrbook.com/a/bookf90pdf.php)

Prerequisites: Basic knowledge of calculus and undergraduate physics; familiarity with a programming language such as C or Fortran.

Course Description
Students will learn basic elements of computational methods and acquire hands-on experience in their practical use in the context of computer simulations to solve physics problems.

Syllabus
1. Monte Carlo (MC) simulation of spins—Ising model
   - Numerical *vs*. MC integration: Simpson's rule, Gaussian quadrature (orthogonal functions—recursive function evaluation, generating functions)
   - Probability: Importance sampling, Markov chain, Metropolis algorithm
   - Random number generation (RNG)
   - Statistics: Variance, standard deviation, standard deviation of the MC mean
   - Cluster analysis: Graphs, search, stack
2. MC simulation of stock price—geometric Brownian motion
   - Random walk: Einstein's law, central-limit theorem
   - Random variable: Black-Scholes analysis
   - Coordinate transformation: Jacobian, Box-Muller algorithm for RNG of normal distribution
   - Interpolation: Least square fit of data
   - Quantum MC and kinetic MC simulations
3. Molecular dynamics (MD) simulation of particles—Newton's second law of motion
   - Numerical differentiation
   - Ordinary differential equation (ODE): Symplectic integrators
   - Minimization of functions: Conjugate gradient method
   - Hybrid MD/MC simulation
4. Quantum dynamics simulation of an electron—time-dependent Schrödinger equation
   - Partial differential equation (PDE)
   - Fourier analysis: Spectral analysis, fast Fourier transform (FFT)
5. Electronic structures of molecules—quantum mechanical eigenvalue problem
   - Linear algebra: Matrix, orthogonal transformation, rank, singular value decomposition, Krylov subspace
   - Matrix eigensystems: Householder transformation, QL decomposition
   - Root finding: Newton-Raphson method

Grading Scheme
Homework assignments (6-7 assignments), 85%; final project, 15%
A (100-90%); A– (90-85%); B+ (85-80%); B (80-75%); B– (75-70%); C (70-60%); D (60-50%)