PHYS 516: METHODS OF COMPUTATIONAL PHYSICS
Spring 2018 (class number: 50614R)

Instructor: Aiichiro Nakano: VHE 610; (213) 821-2657; anakano@usc.edu

Lecture: 9:00-9:50 am M W F, KAP 138

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, Fortran 77: www.nrbook.com/a/bookfpdf.php, or Fortran 90: 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%)