

PHYS 516: METHODS OF COMPUTATIONAL PHYSICS

Spring 2022 (section: 50614R)

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TA: TBA
Lecture: 9:00-9:50 am M W F, KAP 145
Office Hour: 4:00-5:50 pm F, VHE 610
Course Page: <https://aiichironakano.github.io/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%)