Syllabus for Physics 5640: Computational Physics II

TEXT: There is no required text for this course. However, *Numerical Recipes* by Press, Tuekolsky, Vetterling, and Flannery (whichever edition) is a standard reference book for algorithms, and it is probably the most useful book you could buy. I highly recommend that you buy a copy, but for this course you could just look at the free version of the older (second) edition at <http://apps.nrbook.com/c/index.html>.

If you already own a copy of *Computational Physics: problem solving with computers* by Rubin H. Landau and Manuel J. Paez (and Cristian C. Bordeianu in the 3rd edition) from a previous course, you might on rare occasions find it useful to look at, but I would not recommend shelling out $$$s for a copy if you don't already have one. There is a copy on reserve in the Physics library.

Finally, there are an assortment of other books on the Physics library reserve shelf for this course, which you could peruse.

Grading:

100% Homework

No Final Exam: There will not be any formal exams in this course. Grading will be based on the homework assignments.

Homework: Will always be due at the **start** of the class in which it is due. There will be significant penalties for late homework..

I encourage you to discuss with other students in the class methods for attacking the problems. I encourage you to discuss debugging difficulties with each other. However, the actual code you write must be *your own from start to finish*, except that you may start with any code that I present in class and post on galileo. You must individually create, write, and run your own code without direct copying from another student or another source. (If I give any non-coding problems, the same applies: you may discuss methods, but you have to write up your own solutions without copying.) Copying would be a serious breach of honor.

Under no circumstances may you copy another student's code—not even to use as a starting point for your own modifications. If you seek help from another student (say, to help you debug your program), that's great—but they shouldn't sit down at the terminal to fix it for you. Advice, help, and ideas are okay; writing code from someone else is not.

Many of the problems that I assign may have been assigned in this class in a previous year. **DO NOT** obtain or look at student or teacher solutions from previous years. That would be a violation of the honor code.

Attendance: You are responsible for the material presented in class, turning in your homework on time, knowing problem assignments, and knowing any administrative announcements made, such as changes to the syllabus or changes to the scheduling of homeworks.

The programming language used in this course will be C. You are welcome to use C++ if you prefer.

Tentative Syllabus for Phys 5640

1. Linear Algebra Methods
– Algorithms for matrix inversion and diagonalization:
Gaussian elimination, backsubstitution, pivoting,
LU decomposition, tridiagonalization
– Singular value decomposition (SVD)
– Sparse matrix methods:
Jacobi and Gauss-Seidel relaxation methods, conjugate
gradient method

2. Partial Differential Equations
– Discretization of PDE's on a lattice
– Hopping matrices, propagators, and random walks
– Heat flow problems and relaxation methods
Jacobi and Gauss-Seidel iteration
– Solving the Schrodinger 3-D bound state problem
by minimization methods
The conjugate gradient algorithm
– Real-time solution of PDE's - Time dependent
Schrodinger equation and application to quantum
mechanical scattering
Unitarity and probability conservation
The Crank-Nicholson algorithm

3. Quantum Theory of Conductivity
– Schrodinger equation in a periodic potential (1D and 2D):
Bloch waves
– Effects of disorder: Anderson localization
– 2d Schrodinger equation in a magnetic field; Bloch waves,
– Anderson localization,
– Schrodinger equation with a magnetic field,
Landau levels
– The integer Quantum Hall Effect

4. Monte Carlo Methods
– Monte Carlo integration
– Partition functions in statistical physics

– Markov chains and the Metropolis algorithm
– Heat bath techniques
– Hybrid methods and detailed balance
– Monte Carlo simulation of spin models in 2-D and 3-D
Seeing phase transition on the computer
– Path integrals in QM and QFT
The stat-mech - QFT connection
Monte Carlo simulation of quantum field theories

5. Integrable Nonlinear Differential Equations
– The Korteweg-Devries Equation
– KdV solitons
– KdV solitons aa reflectionless potentials
– Connection between KdV equation and Schrodinger equation
The "inverse scattering" transform

6. Advanced Methods for Solving Linear Algebra Problems
– Theory of the conjugate gradient method
Orthogonal directions and conjugate directions
Bi-orthogonalization
– Krylov subspaces
– Methods for solving eigenvalue problems
Lanczos method
Ritz method
Tridiagonalization of matrices

7. Special Topics in Computational Physics
– Exploring statistical mechanics, field theory, condensed matter physics,
and particle physics with computer intensive methods