PHY 3301H — COMPUTATIONAL METHODS IN THE PHYSICAL SCIENCES

Spring 2005
BH 1610
MW: 3.00 p.m. – 4.40 p.m.

Instructor: Sergey Buldyrev
buldyrev@bu.edu
Belfer 1112
Extension: 430

Office Hours: MW: 5:00 p.m. – 6:00 p.m.

Required Texts:

Numerical Recipes in C, by W. H. Press *et al*., ISBN:0-521-43108-5
Computational Physics, by J. M. Thijssen, ISBN:0-521-57588-5

Supplementary Texts:

The C programming Language, by B.W. Kernighan and D. M. Ritchie
ISBN: 0-13-110370-9

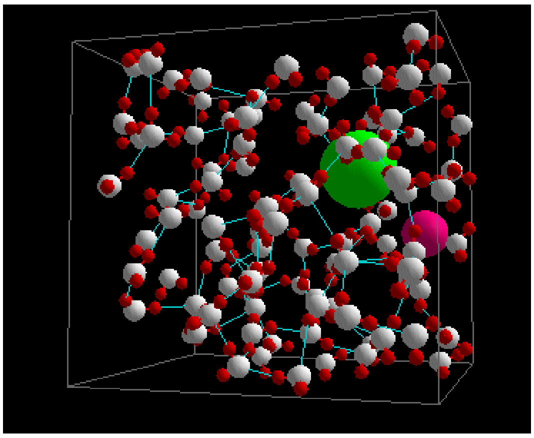
Grading:

Homework and class participation	40%
Periodic computational projects	40%
Final computer project	20%

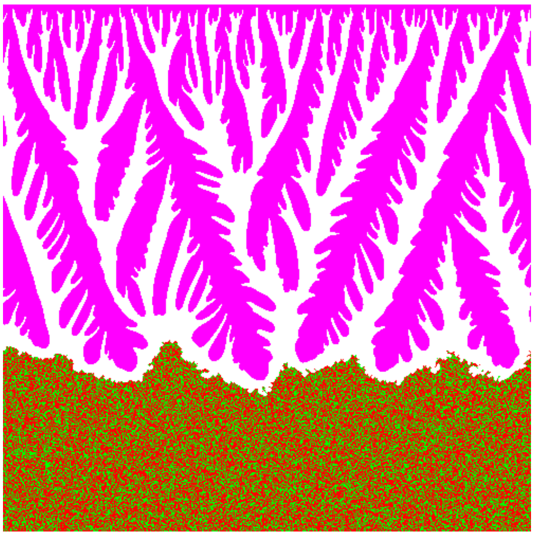
Course Summary:

This hands-on course will explore how a computer can help us try to explain how the natural world functions. After a brief introduction to basic computing, we will discuss concrete problems drawn mainly from Physics but also from Chemistry, Math, Biology, and Computer Science, examining in each case how we can use computers to model the problem and explore it quantitatively. The problems will include some of my own interests and may come to include some of yours. Physicists have known the analytic solutions to some problems for centuries (planetary motion, for instance), but we will also look at problems which have come to the forefront of science only in the last few years (e.g., chaos, growth of structures by deposition, spread of diseases by physical contact, behavior of large biological molecules such as proteins), as well as at problems to which the computer can afford us some hints of a possible solution although an analytic solution does not yet exist (e.g., the Ising model for ferromagnetism in dimensions greater than two). One of the main goals will be covering a broad range of computational methods applicable to many fields. These methods will include numerical solution of algebraic and differential equations (ordinary and partial), boundary problems, interpolation, statistical and spectral analysis, optimization, Monte-Carlo and Molecular dynamics.
You will also accuire very useful programming skills including Mathematica, C and C++.

Prerequisites: Year of calculus AND year of physics OR year of computer science OR permission of the instructor.
Requirements: periodic smaller computational projects and a final larger project which will involve using a supercomputer cluster which I am going to build. Some projects (see examples below) will deal with problems of current scientific interest and may be extended as work-study research during summer.



Molecular dynamic simulations of an ionic solution are based on numerical integration of ordinary differential equations of motion .



Simulations of dendritic crystal growth are based on numerical integration of a partial differential equation.

Course Schedule:

Dates	Topic	Textbook Ch.
January 26	Introduction, C/C++	K&R
February 2	Root Finding and Fractals: Iteration/Bisection/Newton	Press, Ch 9, Th, A3
February 7	Logistic Equation, Period Doubling, Chaos	Press, Ch 9
February 9	Mandelbrot Set, Self-Similarity	Press, 9
February 14	Integration: Rectangles, Simpson, Examples from Physics	Press, 4.2
February 16	Ordinary Differential Equations, Pendulum	Press, 16.1
February 21	Two Body Problem	
February 23	Three Body Problem	
February 28	Double Pendulum, Strange Attractors	Th A7

March 2	Molecular Dynamics: Leapfrog method	Th 8
March 2	Molecular Dynamics: Neighbor Lists	Th 8
March 7	Discret Molecular Dynamics	
March 9	Sorting: Quick Sort, Bubble Sort, Tree Sort	Press, 8
March 14	Finding words in the Bible, Zipf Law	K&R 6.5
March 16	Introduction to Monte Carlo Method	Th 10.
March 21	Random Number Generators	P 7
March 23	Simulated Annealing	P10.9
March 28	Random Walk	Th10
March 30	Diffusion Limited Aggregation	Th10
April 4	Self-Avoiding Random Walk	Th10
April 6	Percolation	Th10
April 11	Ising Model	Th10
April 13	Wang-Swendsen Method	Th10
April 18	Solving Linear Equations, curve fitting	P1,P2
April 20	Eigenvalue problems	P11
May 4	Partial Differential Equations	P19
May 9	Boundary Problems	P19
Presentations of the Final Projects		