Syllabus of Computational Physics (PHZ 5156)

Instructor: Dr. Pedro Marronetti
Charles E. Schmidt College of Science
Room SE 440. (297-3386)
pmarrone@fau.edu

Classes: MWF / 9:00 – 9:50 AM. Classroom: SE 102

Office Hours: MWF / 9:50 – 12:00PM

Course Website: Blackboard Assigned

Assessment Procedures: The final grade will be determined by the successful completion of all the homework assignments (80% of the final grade) and a Final Project (20%), to be presented during the last week of classes. The deadline for all the homework assignments is April 26, 2007 (Reading day). The project's subject and tentative goals will be chosen by the student's adviser (whenever applicable), among numerical problems that are typically present in their corresponding area of research.

Introduction

The goal of Computational Science is to assist the scientist with numerical methods to attack problems where the lack of analytical solutions or the complexities of a particular model make any other alternative impractical. Solving differential equations, exploring large parameter spaces, or simulating physical systems through the generation of random events are some examples of the most common uses of computers in scientific research. This course will cover numerical methods currently used to address such mathematical problems as well as the programming techniques associated with them.

The different methods studied in the course will be applied to typical problems of Physics. However, **no background in Physics is required for this course**. The techniques can easily be ported to similar problems found in any other area of science and engineering. Basic programming skills (in either C or FORTRAN) are **required**.

The theoretical study of the algorithms will be complemented with comprehensive programming assignments that will allow the students to become familiar with the practical implementation of these techniques.

The course will cover the following subjects:

- Error, Precision, and Stability in Computational Science

- Numerical Integration: Trapezoidal, Simpson, Bode rules. Open and Semi-open formulas. Gaussian quadratures
- Interpolation, Extrapolation and Data Fitting: Polynomial interpolation, Neville's algorithm. Cubic spline. Data fitting, least-squares fits.
- Deterministic Randomness: Random number generators, Linear congruent method. Random walk. Non-uniform distributions of random numbers: exponential, Gaussian and arbitrary distributions. Von Neumann rejection method.
- Monte Carlo Methods: Integration by rejection, integration by Importance Sampling, integration by Von Neumann rejection.
- Root Finding and Equation Solving: Bracketing. Bisection, Secant, False Position, Brent, Newton-Raphson Methods. Root-finding in many dimensions.
- Systems of Linear Equations: Gauss-Jordan elimination. L-U Decomposition. Eigenvalue problems.
- Commercial Subroutine Libraries: Math libraries. Compiling and linking. Code optimization.
- Derivatives using Finite-Differences: Stencils. One-sided differences. First, second and mixed derivatives.
- Ordinary Differential Equations (ODEs): Order reduction. Boundary conditions. Euler method. Runge-Kutta method. Examples: Non-linear oscillator, Schrödinger Equation, Numerov's method. Adaptive Stepsize control. Richardson extrapolation. Bulirshc-Stöer method.
- Partial Differential Equations (PDEs): Classification: hyperbolic, parabolic and elliptic equations. Initial vs. Boundary value problems.
- Hyperbolic Equations and Flux Conservative Methods: Von Neumann stability analysis. Courant-Friederichs-Lewy condition. Euler (FTCS) method. Lax method. Staggered Leapfrog method. Two-Step Lanx-Wendroff method. Phase, non-linear and transport errors.
- Parabolic Equations and the Diffusion Problem: Fully Implicit method. Crank-Nicholson method. Time-dependent Schrödinger Equation: Cayley's method, Operator Splitting.
- Elliptic Equations: Relaxation vs. Rapid methods. Jacobi method. Gauss-Seidel method. Succesive Overrelaxation (SOR). Multigrid methods.
- Fourier Transforms : Properties. Convolution and Correlation. Discrete Sampled Data: Sampling Theorem, Discrete Fourier Transform. Fast Fourier Transform (FFT).

Bibliography

Computational Physics: Problem Solving with Computers
R. H. Landau and M. J. Páez
http://www.physics.orst.edu/%7Erubin/CPbook/index.html

Numerical Recipes: The Art of Scientific Computing
W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery
http://www.nr.com