Syllabus of Introduction to Scientific Programming (PHY 4936/ PHY 5937)

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Classes: TR / 9:00 – 10:20 AM. Classroom: BU401

Office Hours: TR / 10:30 – 12:00 PM

Course Website: Blackboard Assigned

Assessment Procedures: Two take home exams (25% of final grade each) and two classroom tests (25% each). Homework assignments will not be graded.

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 introduce some of the basic tools of scientific programming to prepare the students for advanced courses in numerical computation. We will cover the Unix/Linux operating system, widely used in the scientific community, with particular emphasis in programming and visualization tools. We will introduce the student to the FORTRAN 90 language as well as its use in high performance programming architectures. The course will also cover parallel programming using the Message Passing Interface (MPI) language.

No background in Physics is required for this course. The programming techniques can easily be ported to any other area of science and engineering.

The course will be held in a computer laboratory, where the students will get real time hands-on experience of the methods and techniques described in class.

The course will cover the following subjects:

- Introduction to Unix
- Error, Precision, and Stability in Computational Science
- Text Editors
- Plotting and Visualization

- FORTRAN
- Parallel Programming
- Message Passing Interface (MPI)
- Commercial Subroutine Libraries
- Code Performance Optimization
- Supercomputers: Introduction
- Supercomputers: Queues, Scripts and Jobs Submission

Bibliography

"Introduction to U nix – Second Edition"
David Schwartz, Prentice Hall New Jersey 2006.

"Introduction to Programming with Fortran"
Ian Chivers and Jane Sleightholme. Springer-Verlag London 2006.

Class notes will be distributed.