

ME 581
Numerical Methods for Engineers and Scientists
Fall 2007, Potter 262, Tu/Th 1:30-2:45PM
Prof. S. H. Frankel

Introduction

Numerical methods, numerical analysis, and scientific computing are all related to the use of a computer to solve problems in science and engineering. This process typically involves the development of a mathematical model, and hence a knowledge and appreciation of the relevant physics underlying the problem of interest and the ability to make pertinent assumptions or approximations to facilitate solution of the problem. The choice of using one numerical method over another is many times related to the inevitable tradeoff between the desired efficiency and the required accuracy of the sought after results. Hence, each numerical method studied will have errors that must be accounted for and understood and advantages (pro's) and disadvantages (con's) that must be considered. As computers become more powerful (that is, they are faster with more memory, which nowadays means parallel supercomputers like the IBM Blue Gene P with 130,000 processors, currently the World's fastest computer - see www.top500.org), the choice of algorithm (and whether it can be used on a parallel computing platform) has become even more important. As a student in this class you will gain invaluable experience with programming a wide range of numerical methods for an equally wide range of mathematical problems (stemming from typical problems in science and engineering) and get a first hand feel for the relative accuracy and efficiency of each of the methods. The experience and excitement of going from mathematical equations to beautiful computer graphics of some complex problem, and everything in between, is unique in science and engineering - after all you are simply manipulating a bunch of 0's and 1's!!!

Course Description

This course offers an introduction to numerical methods in science and engineering. Only background in college level mathematics, e.g. calculus and linear algebra and introductory computer programming, is required. The course will cover everything from root finding to solving systems of equations, to finding eigenvalues and eigenvectors, to interpolation of data or functions, to differentiation and integration of functions, to solving ordinary and partial differential equations. Exposure to modern programming languages, such as Fortran90, the Linux operating system, and various open-source Linux packages used for scientific computing and technical report writing, e .g. vi, LaTeX, octave, ..., as well as to advanced computer graphics visualization software packages, e. g. gnuplot, xmgrace, Tecplot, ..., is also featured.

Textbook

“A Friendly Introduction to Numerical Analysis” by Brian Bradie, Prentice-Hall, 2006.

Course Topics:

Below is an itemized list of the main topics to be covered in this class with the approximate number of classes allotted.

- Introduction to Numerical Methods (1 class)
- Introduction to Fortran90 (1 class)
- Root Finding (3 classes)
- Systems of equations (7 classes)
- Eigenvalues and eigenvectors (3 classes)
- Interpolation (3 classes)
- Differentiation and Integration (3 classes)
- Ordinary differential equations (4 classes)
- Partial differential equations (4 classes)

Homework, Computer Projects, and Reporting

You will be given reading and homework assignments every few lectures taken from the textbook or outside sources. The amount of computer programming assignments will increase after the first few weeks of the semester. Hence, please use the first few weeks to brush up on or learn Fortran90 programming (suggested references will be mentioned in a special lecture). Several of your early homework assignments will involve writing simple programs and graphing the results to help you prepare for the later computer programming assignments and get used to the computing environment (discussed below). The computer programming will involve writing your own computer code from scratch. There are a lot of programs available on the Internet and you may be tempted to try and find one that matches the requirements of the assignment - but please resist the temptation. If you are caught trying to pass off someone else's work for your own you will get a grade of zero for that assignment and your name may be turned over to the Dean of Students for consideration of further punitive action. That said, web searches to learn more can and should be a complement to class work and you are encouraged to discuss the numerical methods and class projects with your fellow students, and of course with me, to help you clarify the material and complete the assignment - but in the end your work must be your own! Some computer programs will also involve writing a short technical report describing the problem being solved, the numerical method being used, your code, and a presentation and discussion of your results. Detailed formatting instructions for this will be provided and electronic submission will be accepted.

Computing Environment

It is highly recommended that you develop, test/debug, run, and post-process all your codes/computer projects using the Unix or Linux environment. Four PCs with the Linux OS (RedHat) installed

have been made available to you. These are physically located in ME 236 with machine names me193pc64.ecn.purdue.edu, me193pc65.ecn.purdue.edu, me193pc66.ecn.purdue.edu, me193pc67.ecn.purdue.edu. You will be able to either sit down in front of these machines (if you are on campus) or logon to these machines remotely through ssh (www.openssh.com). For those of you who are new to Unix/Linux a nice Unix tutorial can be found at: <http://www.ee.surrey.ac.uk/Teaching/Unix/index.html>. I recommend the vi text editor for development and a nice tutorial can be found at: <http://heather.cs.ucdavis.edu/matloff/UnixAndC/Editors/ViIntro.html>. I will recommend some reference books on Linux in class. For much, much more Google is your friend!

Course Grade

Your course grade will be based on your homework, which will be fully or partially graded, for 50%, an in-class closed book/notes midterm for 25%, and a closed book/notes final exam (during final exam week) for 25%. A straight curve or better will be applied to convert your numerical grade to a letter grade.