Project Proposal for Computational Physics Course

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1 Topics

This is the project proposal that I can do for my computational physics course.

• At the first step of my project LU decomposition can be done to solve a system of equations

$$-x_1 + x_2 - 4x_3 = 0 \tag{1}$$

$$2x_1 + 2x_2 = 1 \tag{2}$$

$$3x_1 + 3x_2 + 2x_3 = \frac{1}{2} \tag{3}$$

It can be solved by standard Gaussian elimination analytically. Thereafter I may compare the analytical results with the numical solutation obtained by using the LU program.

• In the next step I may try to solve the one dimensional Poisson equation with boundary conditions by rewriting it as a set of linear equations. We can rewrite the equation as

$$-u''(x) = f(x), x \in (0,1), u(0) = u(1) = 0.$$
(4)

Then we can define the discritized approximation to u as v_i with grid points $x_i = ih$ in the interval from $x_0 = 0$ to $x_{n+1} = 1$. The step length spacing is defined as h = 1/(n+1) with boundary conditions $v_0 = v_{n+1} = 0$. The approximate 2nd dervative of u can be written as,

$$-\frac{v_{i+1} + v_{i-1} - 2v_i}{h^2} = f_i,$$
(5)

for i=1,....,n .where $f_i = f(x_i)$. This equation can be written as a set of linear equations of the form Av = b, where A is an n X n tridiagonal matrix and $b_i = h^2 f_i$. In my case I will assume that $f(x) = (3x + x^2)e^x$, and keep the same interval and boundary conditions.

• The matrix A can be rewritten interms of one-dimensional vectors a,b,c of length 1:n. The tridiagonal system can be written as

$$a_i v_{i-1} + b_i v_i + c_i v_{i+1} = b_i \tag{6}$$

for i=1,2,...,n. Then first I will try to set up the algorithm for solving this set of linear equations and also try to find the no. of operation needed to solve the above equations. Then will try to compare this with standard Gaussian elimination. Then the above matrix can be coded for n=10,100,1000 grid points. Then I will try to compare these result with analytic result for different no. of grid points (different step lengths) in the specific interval. The maximal relative error in the data set (i=1,...,n) can be computed by setting up

$$\epsilon_i = \log_{10}(|\frac{v_i - u_i}{u_i}|) \tag{7}$$

as function of $log_{10}h$ for the function values u_i and v_i . For each step length we can extract the max value of relative error. Then the n value can be increased to $n = 10^4$ and $n = 10^5$.

• By taking n=100(say)we may compare the results, time needed with those form LU decomposition codes and the tridiagonal solver codes.