Elementary Numerical Analysis

2008 년 2 학기

HW#6: 2-D Particle Diffusion

Due Nov. 4, 2008

In this problem set, you are going to find the behavior of the numerical solution of the 3-D particle diffusion given by:

$$-D\left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}\right)+\alpha\phi(x,y)=s(x,y),\quad x\in[0,a],\quad y\in[0,b] \qquad (1)$$

with the following boundary conditions:

$$\left.\frac{\partial\phi}{\partial x}\right|_{x=0}=0,\quad \phi(a,y)=0,\quad \left.\frac{\partial\phi}{\partial y}\right|_{y=0}=0,\quad \phi(x,b)=0$$

The physical constants are given as follow:

$$a=b=5\,cm$$
$$D=2.5\,cm$$
$$\alpha=0.15\,cm^{-1}$$
$$s(x.y)=1000\ particles/cm^3\ /\mathrm{sec}$$

The basic mesh size is 0.5 cm in all directions. We are going to obtain the particle distribution ϕ.

A. Discretization

The meshes are ordered in the natural way, namely, from the upper left corner to the lower right corner. Write a MATLAB program to discretize the 2-D problem and construct the linear system which consists of 100 equations. For sparse storage, use the function *sparse* in MATLAB. Use a sparse matrix storage scheme if you use other language.

B. Reference Solution

Use you LU factor function and solver to generate the reference solution. Plot the radial particle distribution using surf. You need to converted the solution vector to a matrix (2-D) for the plot.

C. Gauss-Seidel Iterative Solution

Write a program to implement the Gauss-Seidel method. Perform the iteration and estimate the spectral radius of the iteration matrix by computing the ratio of pseudo error norms at each iteration step. Namely,

$\rho = \dfrac{\left\| x^{(k)} - x^{(k-1)} \right\|}{\left\| x^{(k-1)} - x^{(k-2)} \right\|}$. Compare this with the theoretical spectral radius which can be obtained by computing the maximum eigenvalue of the spectral radius of the iteration matrix. Exit the iteration when the relative change of the pseudo error becomes less than 10^{-6}. The relative pseudo error is defined as:

$$\tilde{\rho} = \frac{\left\| x^{(k)} - x^{(k-1)} \right\|}{\left\| x^{(k)} \right\|}.$$

D. SOR Iterative Solution

Change the Gauss-Seidel code to a SOR code which implement elementwise extrapolation. Increase the over-relaxation parameter (w) from 1 with a step size of 0.1 until observe an increase in the estimated spectral radius. If there is a turn-over of the estimated spectral radius, step back one step and refine the step size by 1/10. Then try to increase w again to determine the optimum w which gives the minimum spectral radius. Compare the number of iterations needed to achieve the same error for the SOR and G-S cases. You can obtain the exact error of an iterate by comparing with the reference solution. Compare the estimated optimum w with that can be determined analytically by using Young's formula.

E. Effect of Mesh Size

Investigate the effect of the mesh size on the convergence of the iteration scheme and also on the memory and computation requirement for the direct method. To begin with use the mesh size of 1cm. Now you may not be able to obtain the maximum eigenvalue of the iteration matrix from MATLAB. Further reduce the mesh size and see what happens to the estimated spectral radius of the Gauss-Seidel iteration scheme.

Sparse Matrix Storage

anz(k) – an 1-D array containing non-zero entries of A. There are nnz nonzero entries. The nonzero entries are stored sequentially sweeping left to right starting from the first row. The column index of each nonzero entry is stored also sequentially in icol.

icol(k) – an 1-D integer array containing the column index of the k-th nonzero entry.

inzl(i) – an 1-D integer array containing the index of the last nonzero entry of row i. It should be declared with 0 as the lower bound and n as the upper bound.

idiag(i) – an 1-D integer array containing the index of the diagonal entry of row i.

Matrix vector product for i-th row:

```
sum=0
for k=inzl(i-1)+1: inzl(i)
    sum=sum+anz(k)*x(icok(k))
end
sum=sum-anz(idiag(i))*x(i)    % to remove the contribution from the diagonal
```