Elementary Numerical Analysis

HW#7: Eigenvalue Problems for 3-D Particle Diffusion

Due Nov. 18, 2008

In this problem set, you are going to solve the matrix eigenvalue problem originating from the following 3-D particle diffusion equation:

$$-D\left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}\right)+\sigma_A\phi(x,y,z)=\frac{1}{\lambda}\sigma_S\phi(x,y,z)$$
$$x\in[0,a],\quad y\in[0,b],\quad z\in[0,c] \tag{1}$$

and

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

The physical constants are given as follow:

$$a=b=100\ cm,\ \mathrm{c = 200\ cm\ for\ 3\text{-}D}$$
$$D=1.0\ cm$$
$$\sigma_A=0.10\ cm^{-1}$$
$$\sigma_S=0.12\ cm^{-1}$$

The basic mesh size is 25 cm in all directions. You are going to obtain the maximum eigenvalue and the corresponding eigenvector.

A. Matrix Eigenvalue Problem

Discretize the Laplacian of the LHS after dividing both sides by D in the same way as the previous homework set to result in the following matrix eigenvalue problem:

$$A\phi=\frac{1}{\lambda}\frac{\sigma_S}{D}\phi=\frac{1}{\lambda}\frac{\sigma_S}{D}I\phi=\frac{1}{\lambda}S\phi \tag{2}$$

where A is a septa diagonal matrix, S is a diagonal matrix, and ϕ is a vector. The equation can be rewritten as:

$$\lambda\phi=A^{-1}S\phi\equiv B\phi. \tag{3}$$

Thus this corresponds to finding the maximum eigenvalue λ of Matrix B.

1. Construct Matrix B using the MATLAB function inv(A)*S. Determine the eigenvalues and the normalized eigenvectors of B using the MATLAB script [U,LAM]=eig(B). Determine the dominance ratio of this system as well.

2. Use the regular power method to find the maximum eigenvalue and the corresponding eigenvector of B. Terminate the iteration when the change in the eigenvalue between two successive values is smaller than 1.0×10^{-6}. Normalize the eigenvector and compare it with the reference solution obtained from Step 1.

B. Inverse Power Method

The matrix eigenvalue problem can be solved by using the inverse power method which will require the solution of a linear system

$$A\phi^{(k)} = \frac{1}{\lambda^{(k-1)}}\frac{\sigma_S}{D}\phi^{(k-1)}. \tag{4}$$

For the solution of the above linear system, suppose that you will use the *Gauss-Seidel* iterative solver you wrote for the previous homework. The iteration to solve Eq. (4) is called inner iteration in that there is one more level of iteration, which is the power iteration, to update the eigenvalue and the RHS of Eq. (4). The power iteration is thus called outer iteration.

1. Implement the inverse power method. For checking the convergence of the inner iteration, use the relative error norm of the two successive iterate vectors and set the convergence criterion to 1.0×10^{-6}. For checking the convergence of the outer iteration, use also the relative norm of the two successive eigenvectors. Make sure that you store the old eigenvector to a separate variable such as *phid* and use the current eigenvector as the initial guess to begin each inner iteration. Set the convergence criterion of the power iteration to 1.0×10^{-5}.

2. During the outer iteration, evaluate the true relative error by subtracting the normalized eigenvector from the reference eigenvector you obtained from A.2. Plot both the true error and pseudo error vs. iteration on a semilog graph. Explain why you would see large difference in the two curves.

3. Estimate the dominance ratio of this system using the pseudo error ratios of power iteration. Compare this estimate with the one determined by the eigenvalue ratios in

A.1.

4. Discuss the advantage of the inverse power method over the regular (direct) power method of A.2.

C. Physical Factors Affecting Dominance Ratio

The dominance ratio will be changed by the material and geometrical properties of the problem. In order to investigate the behavior of the dominance ratio, examine the following:

1. Increase and decrease the diffusion coefficient by a factor of 2 and 1/2.

2. Now increase and decrease the problem dimensions of the reference problem by a factor of 2 and 1/2. Keep the same number of meshes.

3. Discuss the dependence of the dominance ratio of the two physical factors.