BBSI: “Lab work” for 6/5/07: Partial Diff. Eqs.

1) **Lattice discretization of the Diffusion Equation: operational details.** Consider simple diffusion on the interval 0<x<L subject to absorbing boundary conditions at x=0,L. Thus, the probability distribution of diffusing particles obeys the 1D Diffusion Equation:

$$\frac{\partial p(x,t)}{\partial t} = D\frac{\partial^2 p(x,t)}{\partial x^2} \qquad [1]$$

with $p(0,t) = 0 = p(L,t)$. [D is the appropriate diffusion constant.] Let the NxN matrix $\mathbf{\Delta^{(N)}}$ be defined as the banded matrix having -2 on the diagonal, 1 on the first band above and below the diagonal, and 0 elsewhere. For example, for N=4:

$$\mathbf{\Delta^{(4)}} = \begin{pmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{pmatrix} .$$

Discretizing $p(x,t)$ into an N-dimensional vector $(p_1, p_2, ..., p_N)^T$ such that $p_j(t) = p(ja,t)$, where $j = 1,2,...,N$ and a is the grid spacing, $a = L/(N+1)$, it can be shown that the discrete analog of Eq. 1 is:

$$\dot{\vec{p}} = \frac{D}{a^2}\mathbf{\Delta}^{(N)}\vec{p} \quad . \qquad [2]$$

Eq. 2 can be directly integrated to give:

$$\vec{p}(t) = \exp(\frac{D}{a^2}\mathbf{\Delta}^{(N)}t)\vec{p}(0) \quad .$$

a) Setting L=1 and N=21, let $p_{11}(0) = 1$ and all other components equal to 0. (This corresponds to placing a particle at the center of the box.) Calculate and plot the time evolution of the probability distribution. [Hint: Use the result of *Lab work 1* to exponentiate the matrix $\frac{D}{a^2}\mathbf{\Delta}^{(N)}t$.]

b) All the eigenvalues of $\mathbf{\Delta}^{(\mathrm{N})}$ are negative. Identify the least negative eigenvalue: call this λ_1 and the corresponding eigenvector $\vec{v}_1$. Show that the approximation

$$\vec{p}(t) \cong \left(\vec{v}_1\right)_{11} \vec{v}_1 e^{\frac{D}{a^2}\lambda_1 t}$$

becomes very accurate after short-time transients die off.

2) **Relaxation Method for solving the 2D Laplace Eq**. Given any analytic function $f(z) = u(x,y) + iv(x,y)$ of a complex variable $z = x + iy$, it can be shown that both *u* and *v* satisfy the 2D Laplace Equation. That is,

$$\frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial y^2} = 0 \qquad [3]$$

and likewise for *v*. [Note: Roughly speaking, an analytic function is one which can be represented as a sum of integral powers of its argument.]

a) Pick an analytic function $f(z)$ (your choice!). Show that $u(x,y) = \mathrm{Re}(f(z))$ satisfies the Laplace Eq. (3); also check that $v(x,y) = \mathrm{Im}(f(z))$ satisfies the same equation.

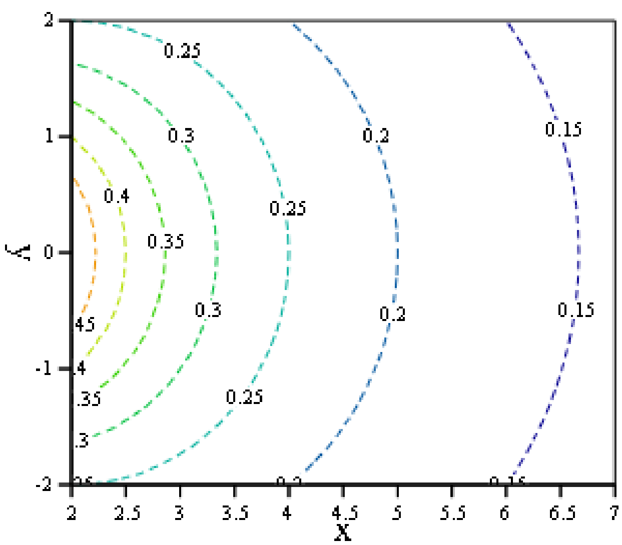

Fig. 1: Contour plot of function $u(x,y) = x/(x^2 + y^2)$, which solves the 2D Laplace Eq.

b) Pick some function that satisfies the 2D Laplace Eq. (e.g., based on part a): denote this as $u(x, y)$ Pick a rectangular perimeter in the x-y plane (again, your choice). [Note: An example is shown in Fig. 1.]

i) Using the known values of u on the perimeter, use the Mathcad subroutine *relax* to compute an approximate solution to the Laplace Eq. in the interior region. (The linear discretization index N is up to you, but check for convergence as described below.)

ii) Make a contour plot of the function computed using *relax* in part i). Compare this to the exact analytical solution obtained in part a). Show that as N is increased, the agreement between the numerical and analytical solutions for $u(x, y)$ improves. (To see the convergence process more clearly, it may be useful to plot $u(x, y_f)$ vs. x, where y_f is a fixed value of y in the interior region.)

3) **Lattice discretization of the Diffusion Equation: derivation.** Returning to problem 1, derive the discretization of the diffusion Eq. [1] that is given in Eq. [2].