

BBSI: “Lab Work” for 6/18/08: 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:

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

with $p(0,t) = 0 = p(L,t)$. [D is the appropriate diffusion constant.] Let the $N \times N$ 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 $(p_1, p_2, \dots, p_N)^T$ such that $p_j(t) = p(ja, t)$, where $j = 1, 2, \dots, N$ and a is the grid spacing, $a = L/(N+1)$, it can be shown that the discrete analog of Eq. 1 is:

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

Eq. 2 can be directly integrated to give:

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

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 $\Delta^{(N)}$ are negative. Identify the least negative eigenvalue: call this λ_1 and the corresponding unit normed eigenvector \vec{v}_1 . Show that the approximation

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

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,

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

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 $u(x, y) = \text{Re}(f(z))$ satisfies the Laplace Eq. (3); also check that $v(x, y) = \text{Im}(f(z))$ satisfies the same equation.

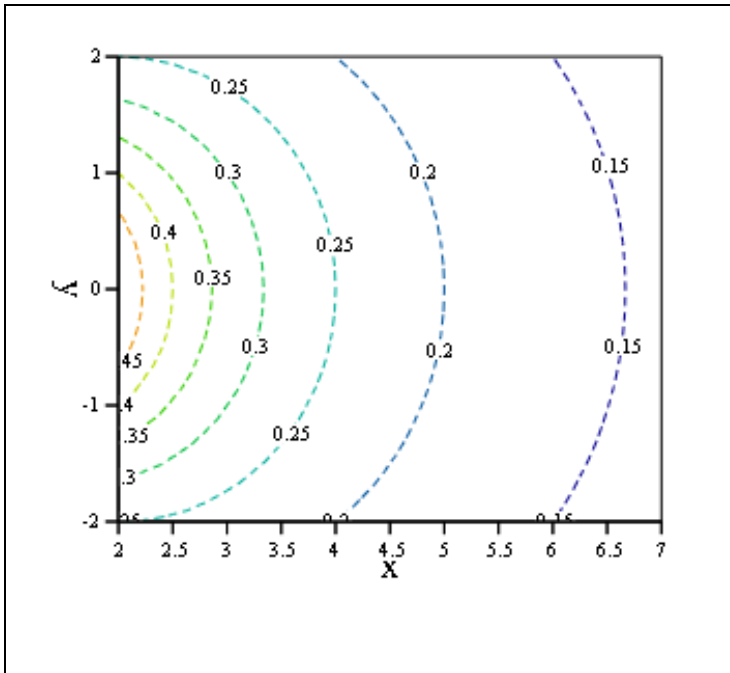


Fig. 1: Contour plot of function $u(x, y) = x / (x^2 + y^2)$, which solves the 2D Laplace Eq.

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].