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:

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

[1]

with \(p(0,t) = 0 = p(L,t)\). [D is the appropriate diffusion constant.] Let the \(N\times N\) matrix \(\Delta^{(N)}\) 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 \(N=4\):

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

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

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

[2]

Eq. 2 can be directly integrated to give:

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

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 \(\frac{D}{a^2} \Delta^{(N)} t\).]
b) All the eigenvalues of $\Delta^{(N)}$ are negative. Identify the least negative eigenvalue: call this $\lambda$ and the corresponding unit normed eigenvector $v$. Show that the approximation

$$p(t) \equiv (v_1)_{11} v_1 e^{\lambda t}$$

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,

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

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].