Department of Applied Mathematics and Statistics
COLORADO SCHOOL OF MINES
MATH484: Capstone - Mathematical and Computational Modeling

Assignment #5, Spring 2015
SOLUTIONS

1. Handout (Lin & Segal) p.31, Problem **2b**
Let $\chi, \mu, D > 0$. Assume that $a(t, x)$ and $\rho(t, x)$ satisfy the nonlinear system of PDEs

$$\frac{\partial a}{\partial t} = \frac{\partial}{\partial x}\left(\mu \frac{\partial a}{\partial x} - \chi a \frac{\partial \rho}{\partial x}\right)$$
$$\frac{\partial \rho}{\partial t} = fa - k\rho + D\frac{\partial^2 \rho}{\partial x^2}$$

Perform a stability analysis of the uniform state $a = a_0 \in \mathbb{R}$ and $\rho = \rho_0 \in \mathbb{R}$ assuming $k = k(\rho)$ and $f = f(\rho)$.

We will use the notation $\hat{a}$ and $\hat{\rho}$ instead of a' and ρ', which is used in the handout. We begin with equations (10) and (11) from the handout and use

$$a(t, x) = a_0 + \hat{a}(t, x)$$
$$\rho(t, x) = \rho_0 + \hat{\rho}(t, x).$$

Upon linearizing the resulting equations, we find

$$\frac{\partial \hat{a}}{\partial t} = \mu \frac{\partial^2 \hat{a}}{\partial x^2} - \chi a_0 \frac{\partial^2 \hat{\rho}}{\partial x^2}$$

for (10), while for (11) more analysis is needed. In particular, this equation becomes

$$\frac{\partial \hat{\rho}}{\partial t} = f(\rho_0 + \hat{\rho})[a_0 + \hat{a}] - k(\rho_0 + \hat{\rho})[\rho_0 + \hat{\rho}] + D\frac{\partial^2 \hat{\rho}}{\partial x^2}.$$

At this point, things become a bit more open-ended, depending upon what you assume about f and k.

Since we don't have any strict information about these functions evaluated at $\rho_0 + \hat{\rho}$, we should approximate. The simplest approximation is to use

$$f(\rho_0 + \hat{\rho}) \approx f(\rho_0), \qquad k(\rho_0 + \hat{\rho}) \approx k(\rho_0).$$

Then, using the fact that the pair (a_0, ρ_0) must be a solution to the original equations, we see that $f(\rho_0)\rho_0 - k(\rho_0)a_0 = 0$, and hence (11) becomes

$$\frac{\partial \hat{\rho}}{\partial t} = f(\rho_0)\hat{a} - k(\rho_0)\hat{\rho} + D\frac{\partial^2 \hat{\rho}}{\partial x^2}.$$

Of course, this is equivalent to the system we investigated in class and the outcome is the same condition, namely

$$\frac{\chi a_0 f(\rho_0)}{\mu k(\rho_0)} < 1.$$

A better idea is to use a first-order approximation

$$f(\rho_0 + \hat{\rho}) \approx f(\rho_0) + f'(\rho_0)\hat{\rho}, \qquad k(\rho_0 + \hat{\rho}) \approx k(\rho_0) + k'(\rho_0)\hat{\rho}.$$

Since we're linearizing the resulting equations, a second-order approximation or greater would merely be eliminated anyway. Again, using the fact that the pair (a_0, ρ_0) must be a solution to the original equations, it follows that $f(\rho_0)\rho_0 - k(\rho_0)a_0 = 0$, and hence (11) becomes

$$\frac{\partial \hat{\rho}}{\partial t} = f(\rho_0)\hat{a} + \left(a_0 f'(\rho_0) - k(\rho_0) - \rho_0 k'(\rho_0)\right)\hat{\rho} + D\frac{\partial^2 \hat{\rho}}{\partial x^2}.$$

Assuming that solutions are of the form

$$\begin{aligned} \hat{a}(t,x) &= C_1 e^{\sigma t}\sin(qx) \\ \hat{\rho}(t,x) &= C_2 e^{\sigma t}\sin(qx) \end{aligned}$$

and using this in the linearized PDEs, we find the system of algebraic equations

$$\begin{aligned} C_1(\sigma + \mu q^2) - C_2 \chi a_0 q^2 &= 0 \\ -C_1 f + C_2(\sigma + k + \rho_0 k' - a_0 f' + Dq^2) &= 0. \end{aligned}$$

This is exactly the linear system

$$\begin{pmatrix} \sigma + \mu q^2 & -\chi a_0 q^2 \\ -f & \sigma + k + \rho_0 k' - a_0 f' + Dq^2 \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

and the only way this can have a non-trivial solution is if the determinant of this matrix is zero. This implies that

$$A\sigma^2 + B\sigma + C = 0$$

where

$$A = 1, \quad B = k + \rho_0 k' - a_0 f' + (D + \mu)q^2,$$

and

$$C = \mu q^2(k + \rho_0 k' - a_0 f' + Dq^2) - f\chi a_0 q^2.$$

The Routh-Hurwitz criterion requires $B > 0$ and $C > 0$ in order to find negative solutions. In order for this to hold for any choice of $q \neq 0$, we must have (from $B > 0$)

$$k + \rho_0 k' - a_0 f' > 0$$

and (from $C > 0$)

$$\mu(k + \rho_0 k' - a_0 f') > f\chi a_0.$$

Since $\mu > 0$, these inequalities can be combined to yield the single condition

$$k + \rho_0 k' - a_0 f' > \max\left\{\frac{f\chi a_0}{\mu}, 0\right\}.$$

2. Handout (Lin & Segal) p.31, Problem **3**
Consider two-dimensional variations so that a and ρ satisfy

$$\begin{aligned}\frac{\partial a}{\partial t} &= \nabla \cdot (\mu \nabla a - \chi a \nabla \rho) \\ \frac{\partial \rho}{\partial t} &= fa - k\rho + D\Delta\rho.\end{aligned}$$

Perform a stability analysis of the uniform state $a = a_0 \in \mathbb{R}$ and $\rho = \rho_0 \in \mathbb{R}$ assuming all parameters are positive constants. Do this by assuming perturbations of the form $\sin(q_1 x + q_2 y + \theta)e^{\sigma t}$ where $q_1, q_2, \theta \in \mathbb{R}$. More specifically, show that if $q^2 = q_1^2 + q_2^2$, then the instability condition remains the same as the one-dimensional case.

We proceed as for the previous problem. First, expressing the equations in terms of directional derivatives, they become

$$\begin{aligned}\frac{\partial a}{\partial t} &= \mu\left(\frac{\partial^2 a}{\partial x^2} + \frac{\partial^2 a}{\partial y^2}\right) - \chi\left[\frac{\partial a}{\partial x}\frac{\partial \rho}{\partial x} + \frac{\partial a}{\partial y}\frac{\partial \rho}{\partial y} + a\left(\frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 \rho}{\partial y^2}\right)\right] \\ \frac{\partial \rho}{\partial t} &= fa - k\rho + D\left(\frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 \rho}{\partial y^2}\right).\end{aligned}$$

Upon linearizing the resulting equations, we find

$$\frac{\partial \hat{a}}{\partial t} = \mu\left(\frac{\partial^2 \hat{a}}{\partial x^2} + \frac{\partial^2 \hat{a}}{\partial y^2}\right) - \chi a_0\left(\frac{\partial^2 \hat{\rho}}{\partial x^2} + \frac{\partial^2 \hat{\rho}}{\partial y^2}\right)$$

for (10), while for (11) this becomes

$$\frac{\partial \hat{\rho}}{\partial t} = f\hat{a} - k\hat{\rho} + D\left(\frac{\partial^2 \hat{\rho}}{\partial x^2} + \frac{\partial^2 \hat{\rho}}{\partial y^2}\right).$$

Assuming that solutions are of the form

$$\begin{aligned}\hat{a}(t,x,y) &= C_1 e^{\sigma t}\sin(q_1 x + q_2 y + \theta) \\ \hat{\rho}(t,x,y) &= C_2 e^{\sigma t}\sin(q_1 x + q_2 y + \theta)\end{aligned}$$

and using this in the linearized PDEs, we find the same system of algebraic equations as in the one-dimensional case, namely

$$\begin{aligned}\left(\sigma + \mu q_1^2 + \mu q_2^2\right)C_1 - \chi a_0\left(q_1^2 + q_2^2\right)C_2 &= 0 \\ -fC_1 + \left(\sigma + k + D\left(q_1^2 + q_2^2\right)\right)C_2 &= 0\end{aligned}$$

with $q^2 = q_1^2 + q_2^2$.

3. Assume $x \in \mathbb{R}$ and use the FTBS method to approximate solutions to the system of PDEs given by (10) and (11) in the handout. In particular, use the spatial interval $[-5, 5]$; constant parameter values $\mu = 1, D = 0.2, f = 0, k = 1, \chi = 10$; and initial conditions

$$a_0(x) = \begin{cases} 2 & \text{if } |x| < \frac{1}{10} \\ 0 & \text{else}\end{cases}$$

$$\rho_0(x) = \begin{cases} 1 & \text{if } x \in [-1.1, -0.9] \bigcup [-3.1, -2.9] \bigcup [-4.1, -3.9] \\ 0 & \text{else} \end{cases}$$

For step sizes use $dx = 0.1$, $dt = 1 \times 10^{-4}$. Create three different figures - a 1×2 matrix of plots with $a_0(x)$ in the left column and $\rho_0(x)$ in the right column, a 1×2 matrix of plots with $a(0.5, x)$ in the left column and $\rho(0.5, x)$ in the right column, and a 1×2 matrix of plots with $a(1, x)$ in the left column and $\rho(1, x)$ in the right column.

The concentration values appear to skew to the left over time and migrate towards the attractant. Below is the associated code.

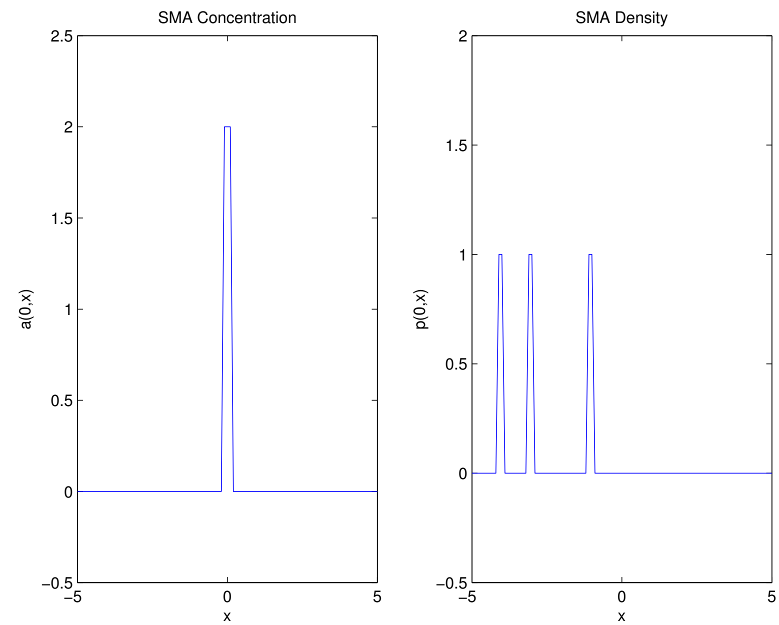

Figure 1: Graphs for Problem 3 at $T = 0$.

MATLAB Code

```
clear; clc;
dx = 1e-1;
dt = 1e-2*dx^2;
a = -5;
b = 5;
T = 1;
x = a:dx:b;
t = 0:dt:T;
n = floor(T/dt);

%Constants
mu = 1;
D = 2e-1;
```

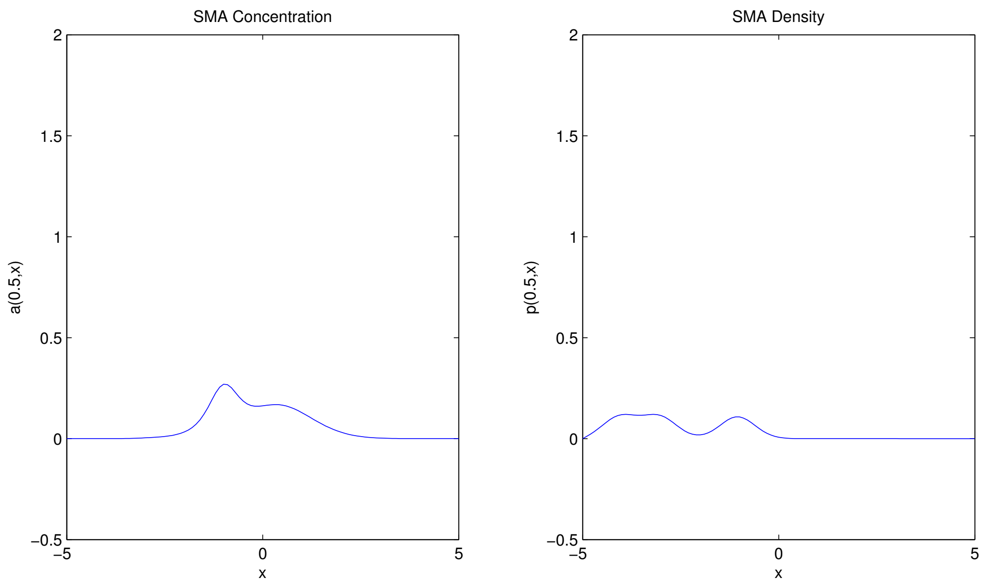

Figure 2: Graphs for Problem 3 at $T = 0.5$.

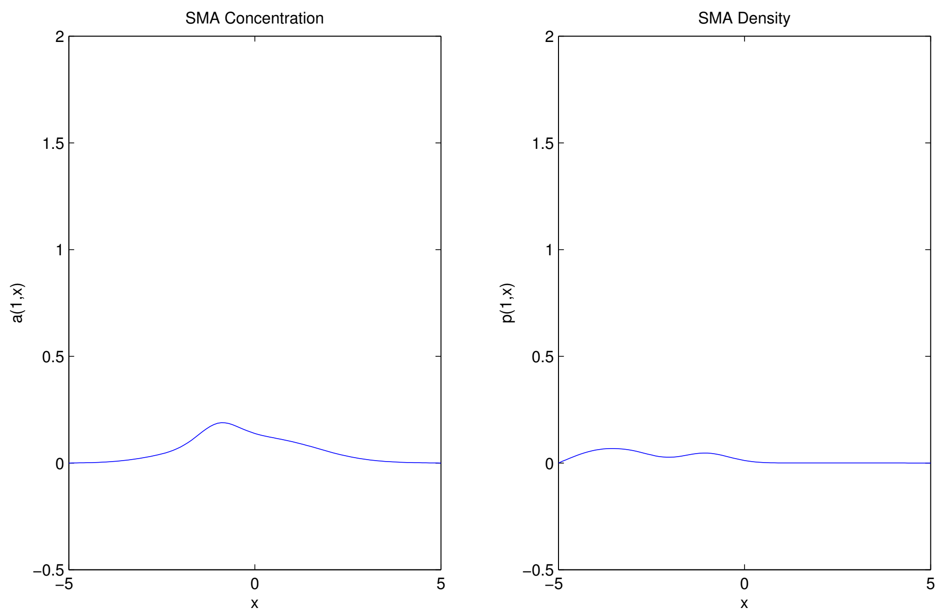

Figure 3: Graphs for Problem 3 at $T = 1$.

```
f = 0;
k = 1;
chi = 10;

%Because a is used for left endpoint, it is replaced by c in code
c(1,:) = zeros(1,length(x));
p(1,:) = zeros(1,length(x));
J1 = find(abs(x) < dx);
```

```
c(1,J1) = 2;
J2 = find((abs(x+1) < dx) |  (abs(x+3) < dx) | (abs(x+4) < dx));
p(1,J2) = 1;

subplot(1,2,1), plot(x, c(1, :)), title('SMA Concentration'),
axis([a,b,-0.5,2.5]), xlabel('x'), ylabel('a(0,x)')
subplot(1,2,2), plot(x, p(1, :)), title('SMA Density'),
axis([a,b,-0.5,2]), xlabel('x'), ylabel('p(0,x)')

for i = 1:n
for j = 2:length(x)-1
c(i+1,j) = c(i,j) +(dt/dx^2)*(mu*(c(i,j+1) -2*c(i,j) + c(i,j-1))...
 - chi*((c(i,j) - c(i, j-1))*(p(i,j) - p(i,j-1))...
  + c(i,j)*(p(i,j+1) -2*p(i,j) + p(i,j-1))));
p(i+1,j) = p(i,j) + dt*(f*c(i+1,j) - k*p(i,j))...
 + D*(dt/dx^2)*(p(i,j+1) -2*p(i,j) + p(i,j-1));
end
end

subplot(1,2,1), plot(x, c(n+1, :)), title('SMA Concentration'),
axis([a,b,-0.5,2]), xlabel('x'), ylabel('a(1,x)')
subplot(1,2,2), plot(x, p(n+1, :)), title('SMA Density'),
axis([a,b,-0.5,2]), xlabel('x'), ylabel('p(1,x)')
```

4. Friedman & Littman, p.53, Problem **3.3.3**
For the equation

$$\partial_t u = \partial_{xx} u$$

use the von Neumann criterion to discuss the stability of the Forward Euler scheme

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2}.$$

Define the constant

$$\sigma := \frac{\Delta t}{(\Delta x)^2} > 0.$$

As in the previous assignment, we begin by using the discrete solution

$$u_j^n = \alpha^n e^{i\beta j}.$$

Multiplying through by Δt, using this solution within the scheme, and dividing by $\alpha_j^n e^{i\beta j} \neq 0$ yields

$$\alpha = 1 + \sigma(e^{i\beta} - 2 + e^{-i\beta})$$

which simplifies to

$$\alpha = 1 + 2\sigma(\cos(\beta) - 1)$$

using Euler's formula. Computing the square and putting the 1 on the left side gives us

$$\begin{aligned} |\alpha|^2 - 1 &= 4\sigma^2(\cos(\beta) - 1)^2 + 4\sigma(\cos(\beta) - 1) \\ &= 4\sigma(\cos(\beta) - 1)\left[\sigma(\cos(\beta) - 1) + 1\right]. \end{aligned}$$

Now, if $\cos(\beta) = 1$ then this becomes $|\alpha| = 1$, which is fine. However, since $\cos(\beta) \leq 1$, the only other option is $1 - \cos(\beta) > 0$, and in this case we must have

$$\sigma(\cos(\beta) - 1) + 1 \geq 0$$

in order for $|\alpha|^2 - 1 \leq 0$. Subtracting the 1 to the right side and dividing by $\cos(\beta) - 1$ which is negative, we find

$$\sigma \leq \frac{1}{1 - \cos(\beta)}.$$

Since we need this to be true for every β, we must impose the condition that σ be less than the minimum of the right side of the inequality, which occurs when $\beta = -\pi$, and this implies

$$\sigma \leq \frac{1}{2}.$$

5. Friedman & Littman, p.54, Problem **3.5.1**
Use a letter of your choice (preferably with a corner or two, and not "L") to create 2 plots - one for the dose $D(x)$ and another containing the backscattered exposure $E(x)$. To create the plot of E, use the parameters $\alpha = \frac{1}{4}$, $\beta = \frac{1}{2}$, and $\eta = \frac{1}{2}$, and implement the Forward Euler method (from Problem 4) to solve the diffusion equation with $dx = dy = 0.05$ and $dt = 2.5 \times 10^{-4}$ on the two-dimensional grid $[-2, 2] \times [-2, 2]$.

The graphs display the effects of the scattering, and the associated code is included below.

MATLAB Code

```
clear; clc;
dx = 5e-2;
dy = dx;
dt = 1e-1*dx^2;
a = -2;
b = 2;

%Constants
alpha = 0.25;
beta = 0.5;
eta = 0.5;
```

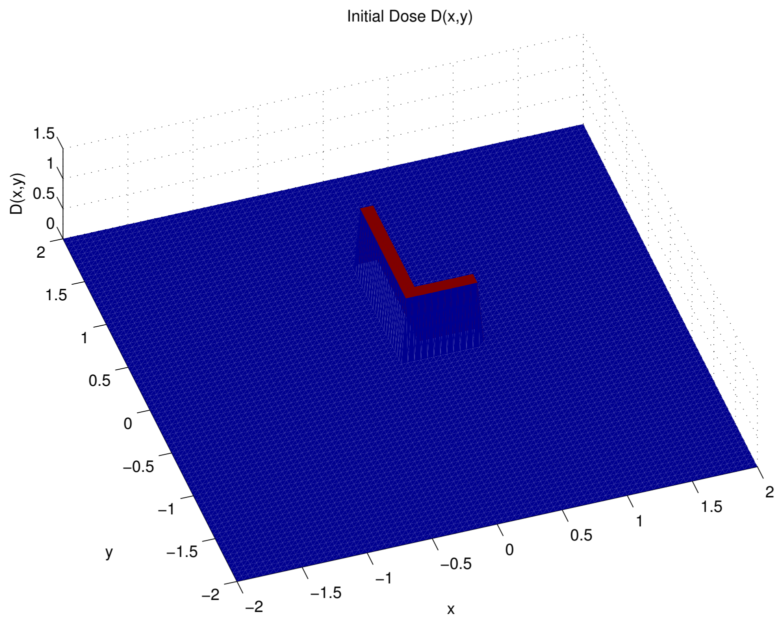

Figure 4: Graph of the dosed "L" region for Problem 5.

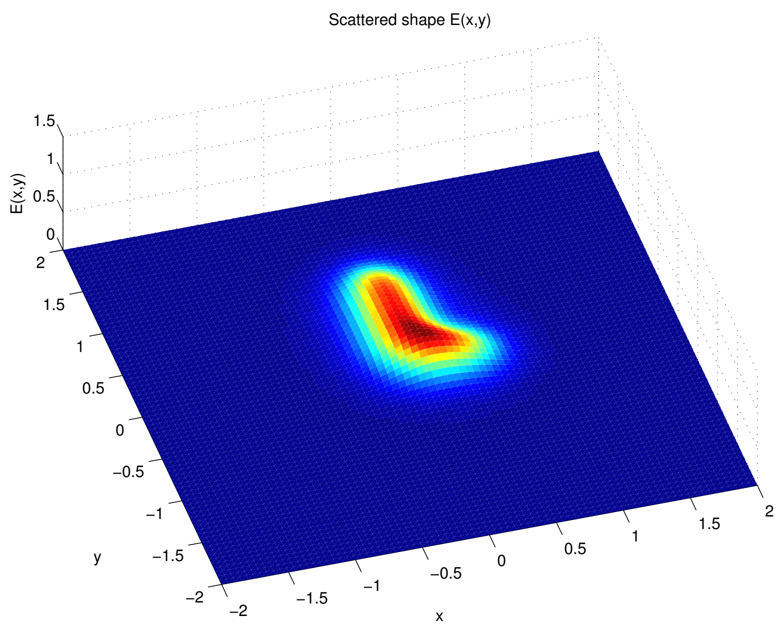

Figure 5: Graph of the scattered shape for Problem 5.

```
T1 = alpha^2/4;
t1 = 0:dt:T1;
n1 = floor(T1/dt);
T2 = beta^2/4;
t2 = 0:dt:T2;
```

```
n2 = floor(T2/dt);
x = a:dx:b;
y = x;

u(:,:,:) = zeros(length(t1)+1,length(x),length(y));

for j = 1:length(x)
    for k = 1:length(x)
        if ((abs(x(j)) <= dx & y(k) >= -dy & y(k) <= 1)...
             | (abs(y(k)) <= dy & x(j) >= 0 & x(j) <= 0.5))
            u(1,j,k) = 1;
        end
    end
end

z = squeeze(u(1,:,:));
surf(x, y, z','EdgeColor', 'none'), title('Initial Dose D(x,y)'),
axis([a,b,a,b,0,1.5]), xlabel('x'), ylabel('y'), zlabel('D(x,y)')

for i = 1:n1
        for j = 2:length(x)-1
            for k = 2:length(y)-1
                u(i+1,j,k) = u(i,j,k)...
                    + (dt/dx^2)*(u(i,j+1,k) -2*u(i,j,k) + u(i,j-1,k))...
                    + (dt/dy^2)*(u(i,j,k+1) -2*u(i,j,k) + u(i,j,k-1));
            end
        end
end

w(1,:,:) = u(1,:,:);

for i = 1:n2
        for j = 2:length(x)-1
            for k = 2:length(y)-1
                w(i+1,j,k) = w(i,j,k)...
                    + (dt/dx^2)*(w(i,j+1,k) -2*w(i,j,k) + w(i,j-1,k))...
                    + (dt/dy^2)*(w(i,j,k+1) -2*w(i,j,k) + w(i,j,k-1));
            end
        end
end

z(:,:) = (1/(1+eta))*(u(n1+1,:,:) + eta*w(n2+1,:,:));

figure;
surf(x, y, z','EdgeColor', 'none'), title('Scattered shape E(x,y)'),
```

```
axis([a,b,a,b,0,1.5]), xlabel('x'), ylabel('y'), zlabel('E(x,y)')
```