BME 7310 Computational Laboratory #5

Due: October 10, 2023

PROBLEM #3. Nerve Transmission Simulations. A firm has decided to award a contract to you for the development of a nerve stimulus transmission software package. Specifically, they want you to solve the **1-D Telegrapher's equation** which is often used in impulse transmission models in nerves. The equation is:

$$\frac{\partial^2 U}{\partial t^2} + \tau \frac{\partial U}{\partial t} = c^2 \nabla^2 U$$

where 'c' is the wave speed, 'U' is potential, and 'τ' is associated with damping. For the numerical scheme, use the following time-splitting scheme and assume second order center difference terms in time:

$$U = \theta\left(\frac{U^{l+1} + U^{l-1}}{2}\right) + (1-\theta)U^{l}$$

where '$l+1$, l, $l-1$' refers to the future time step, the current time step, and the previous time step, respectively. You are going to solve this on a uniformly spaced 1-D grid, i.e. equal spatial steps in 'x'.

a) To accomplish this, you will begin by reporting the *fully discretized molecule equations for a general* ***interior node*****,** and *a node on each boundary* subject to the boundary conditions below:

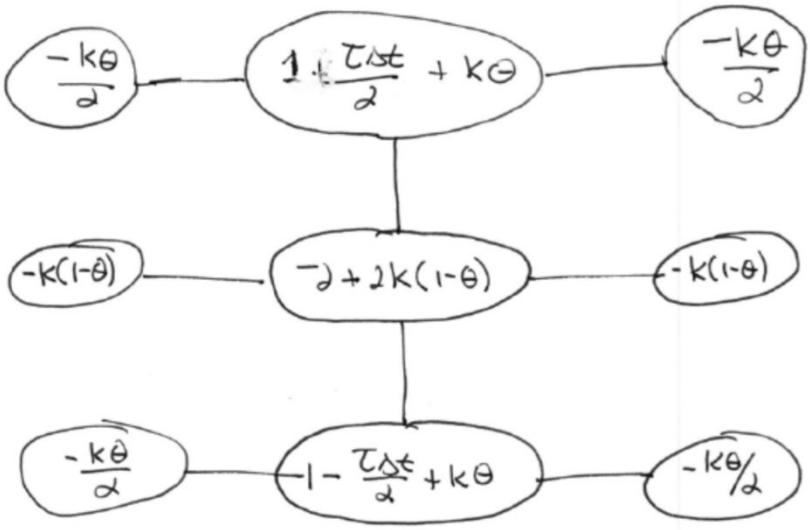
(i) $$\frac{\partial U}{\partial t} - c\frac{\partial U}{\partial x} + \frac{\tau U}{2} = 0 \quad \text{for } x = 0$$

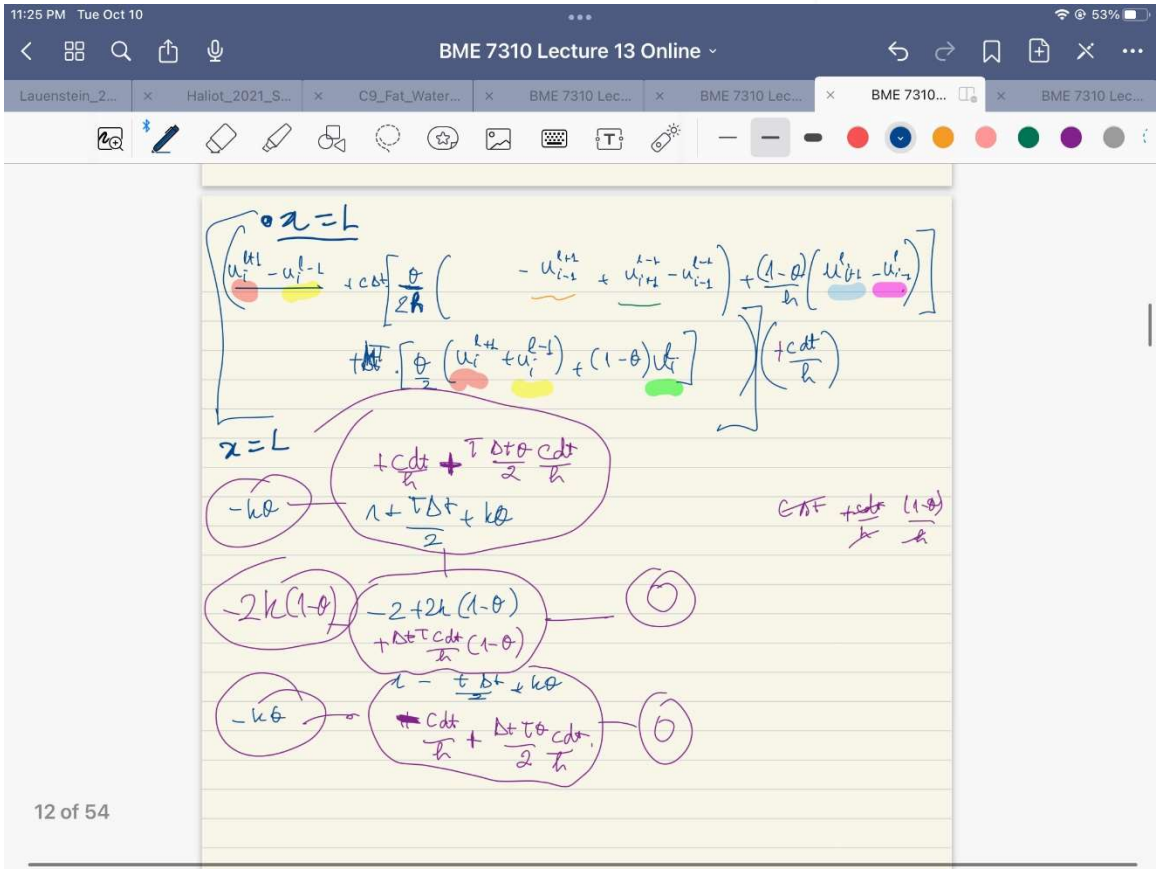
(ii) $$\frac{\partial U}{\partial t} + c\frac{\partial U}{\partial x} + \frac{\tau U}{2} = 0 \quad \text{for } x = L_x$$

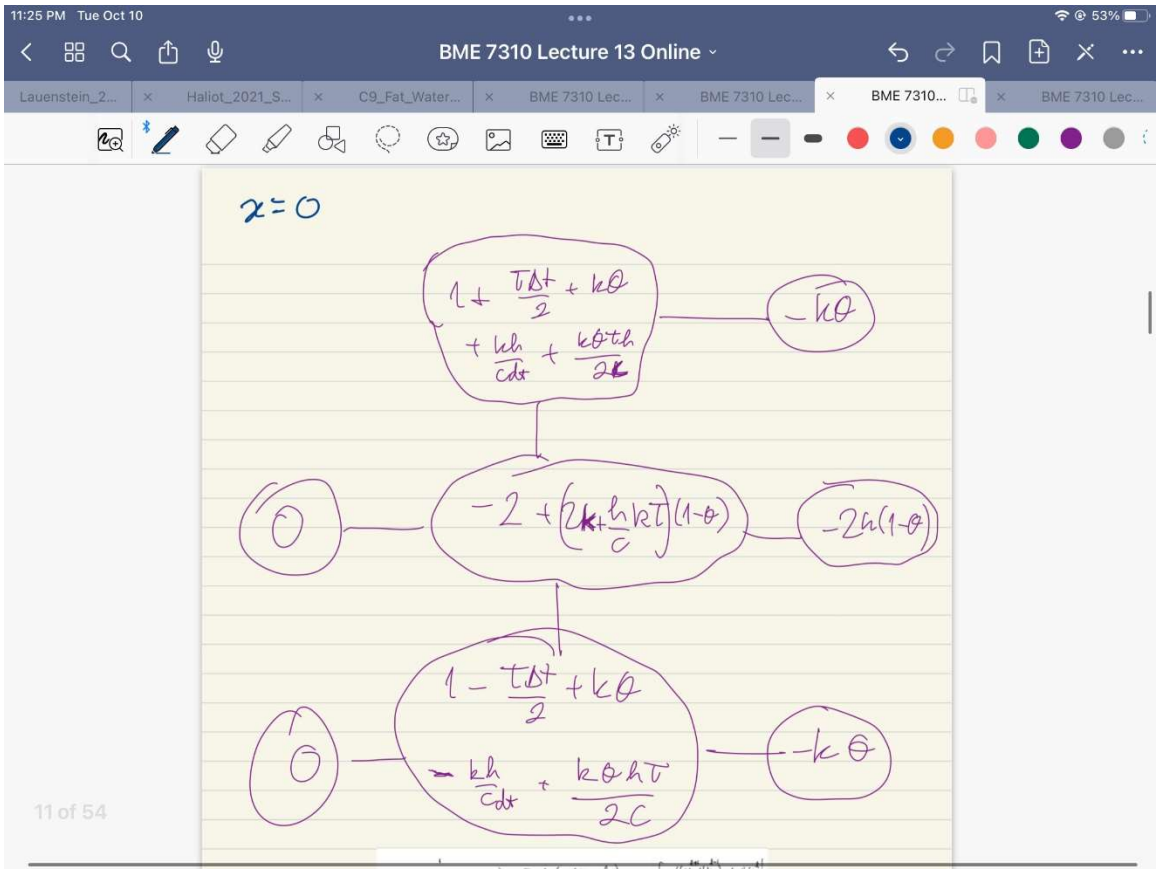
Be sure to explicitly write out how boundary conditions (i), and (ii) will be implemented. Be sure to address their spatial and temporal components. For reference, boundary conditions (i) and (ii) are known as *open boundary conditions*. Their purpose is to let a propagating ***30 mv*** action potential waveform pass through the boundary as though it (i.e. the boundary) were not even there. This type of situation arises when studying physical problems which have domains that extend to infinity or are very long as in the case of nerve fibers. In practice, the mesh must be **truncated at some point which creates a fictitious boundary** with respect to the physical problem and it is desired to have the numerical solution "pass through" the **artificial termination of the computational domain**. In developing your molecules for these boundaries, you will need to extend beyond the standard Type III boundary condition for this case.

$$\left(u_i^{l+1} - 2u_i^{l} + u_i^{l-1}\right) + \frac{\tau\Delta t}{2}\left(u_i^{l+1} - u_i^{l-1}\right) - k\delta_x^2\left[\theta\left(\frac{u_i^{l+1}+u_i^{l-1}}{2}\right) + (1-\theta)\left(u_i^{l}\right)\right]$$

$k=c^2\Delta t^2/h^2$







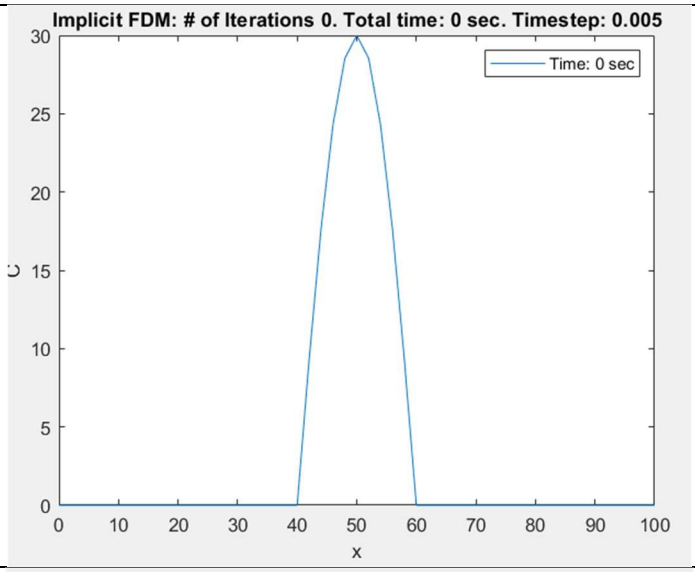
b) Now, code it up. For the sake of a sample problem on somewhat biological scales, let's begin with L_x=100cm, c=9.905 cm/s, τ=0.05/s and the ***30 mv*** initial condition of

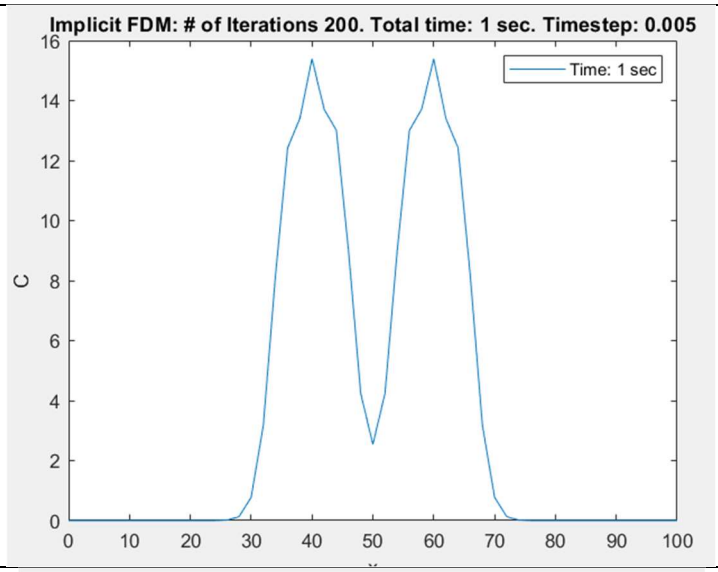
$$U(x,t=0)=30\cos\left(\frac{\pi r}{2r_o}\right) \text{ for } r \le r_o, \text{and } U(x,t=0)=0 \text{ for } r \ge r_o$$

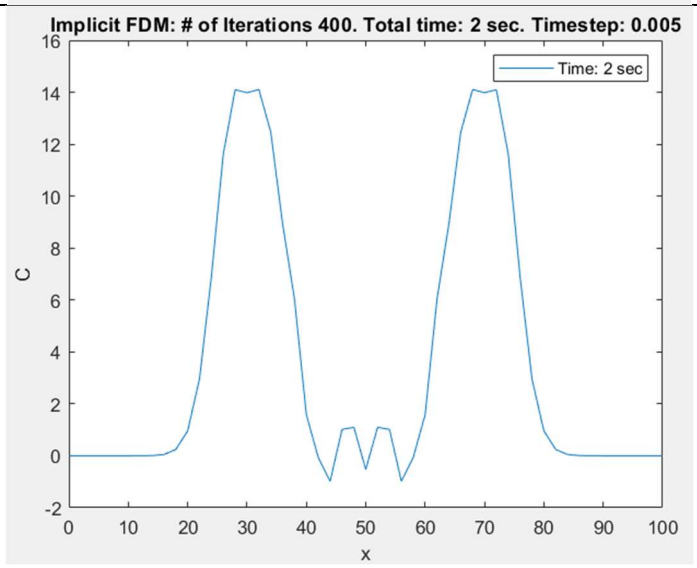
where r_o is the radius of a prescribed circle centered (x_o) and $r=\sqrt{(x-x_o)^2}$, compute the solution to this problem when $r_o=10$cm and x_o=50cm and with dx=2cm for the grid, and θ=0.5 with a time step of dt=0.005 sec. Solve this problem using whatever **direct or iterative method** you wish to compute the matrix solution needed to advance the solution at each time step (i.e. because the discretization scheme is **'implicit'** you will need to solve a spatially coupled system to advance at each time step). With respect to output from your code:

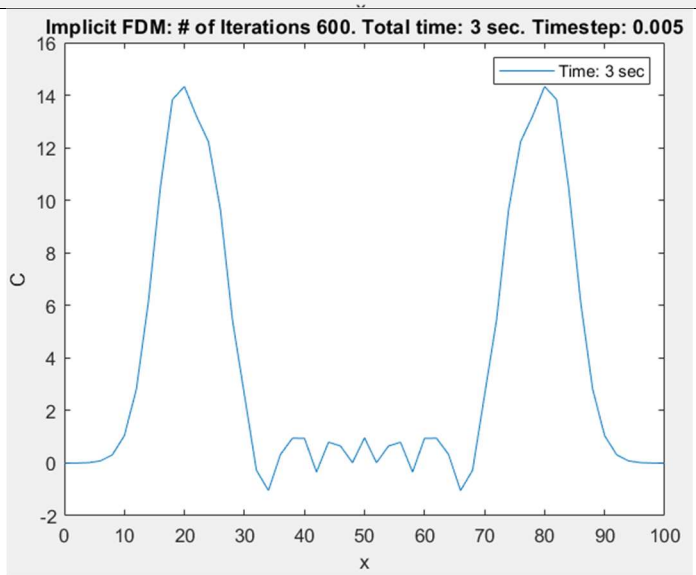
Answer:

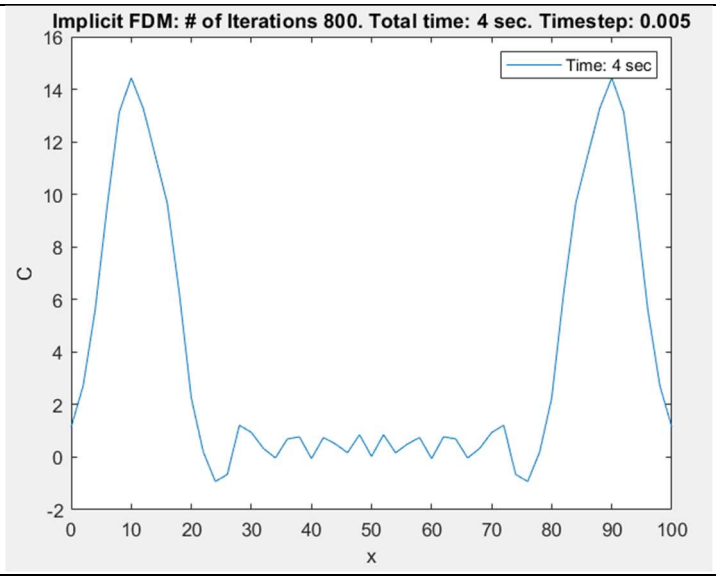
(1) Plot the solution at **every second over the interval 0≤ t ≤10 seconds**,
Here Jacobi Tol=1e-5:

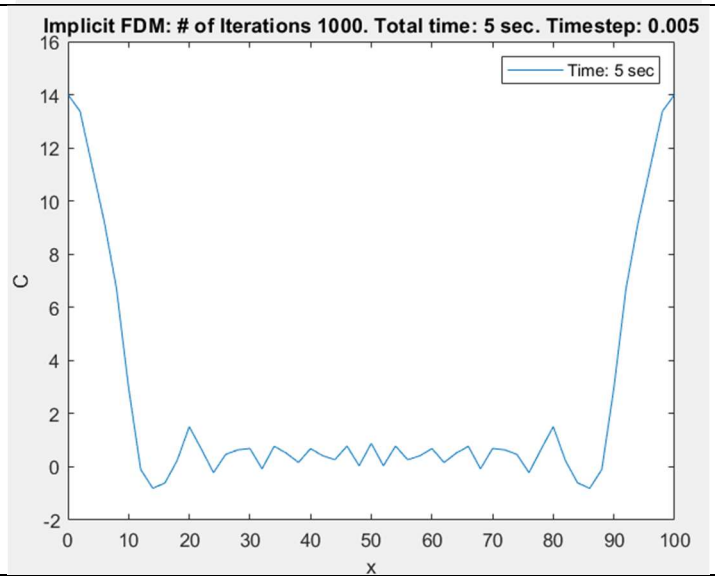

Implicit FDM: # of Iterations 0. Total time: 0 sec. Timestep: 0.005
Time: 0 sec
C
x

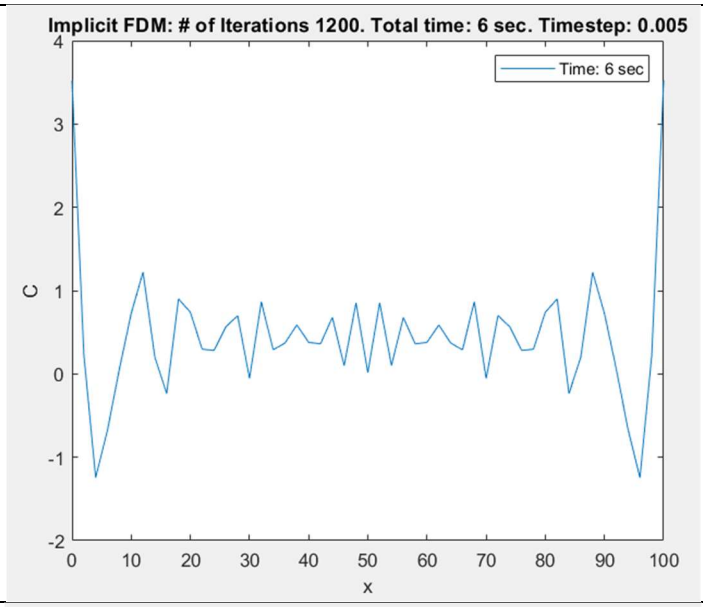

Implicit FDM: # of Iterations 200. Total time: 1 sec. Timestep: 0.005
Time: 1 sec
C
x

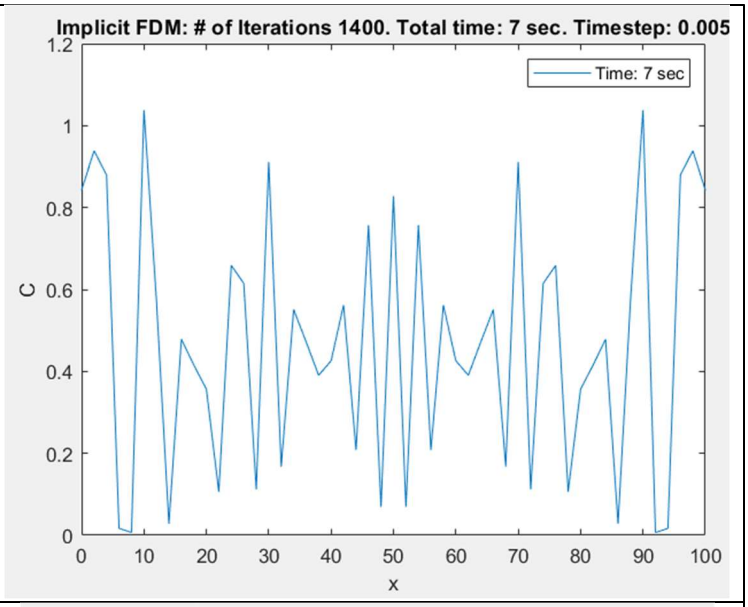

Implicit FDM: # of Iterations 400. Total time: 2 sec. Timestep: 0.005
Time: 2 sec
C
x

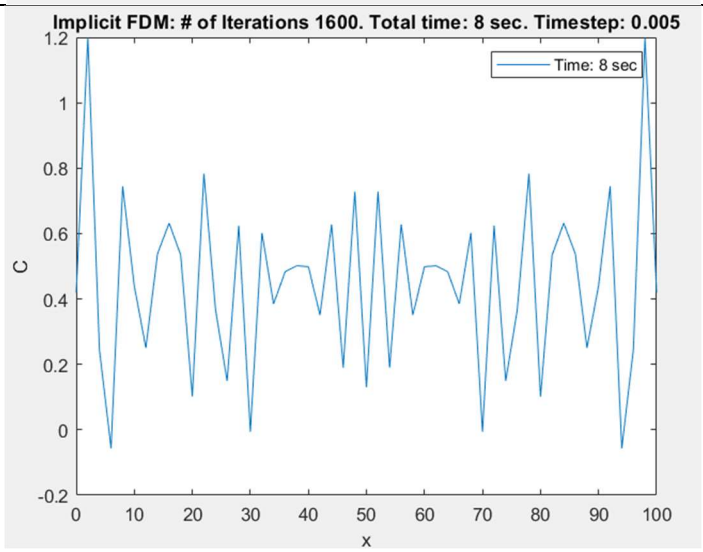

Implicit FDM: # of Iterations 600. Total time: 3 sec. Timestep: 0.005
Time: 3 sec
C
x

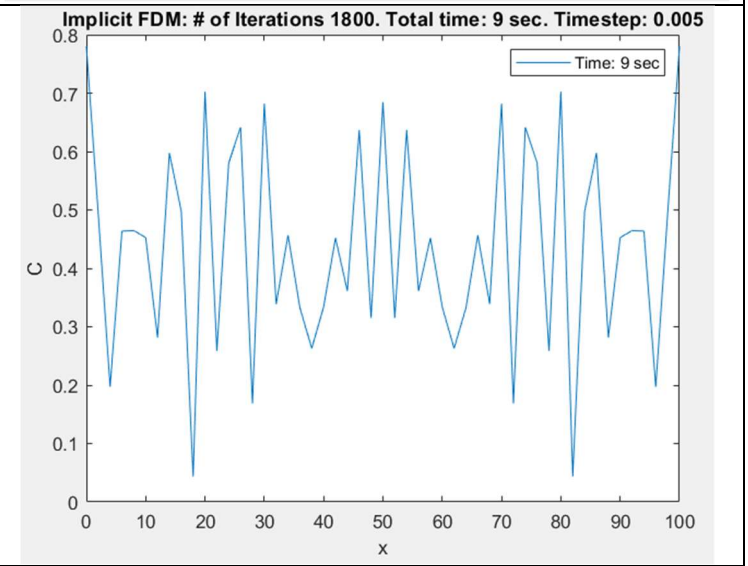

Implicit FDM: # of Iterations 800. Total time: 4 sec. Timestep: 0.005
Time: 4 sec
C
x

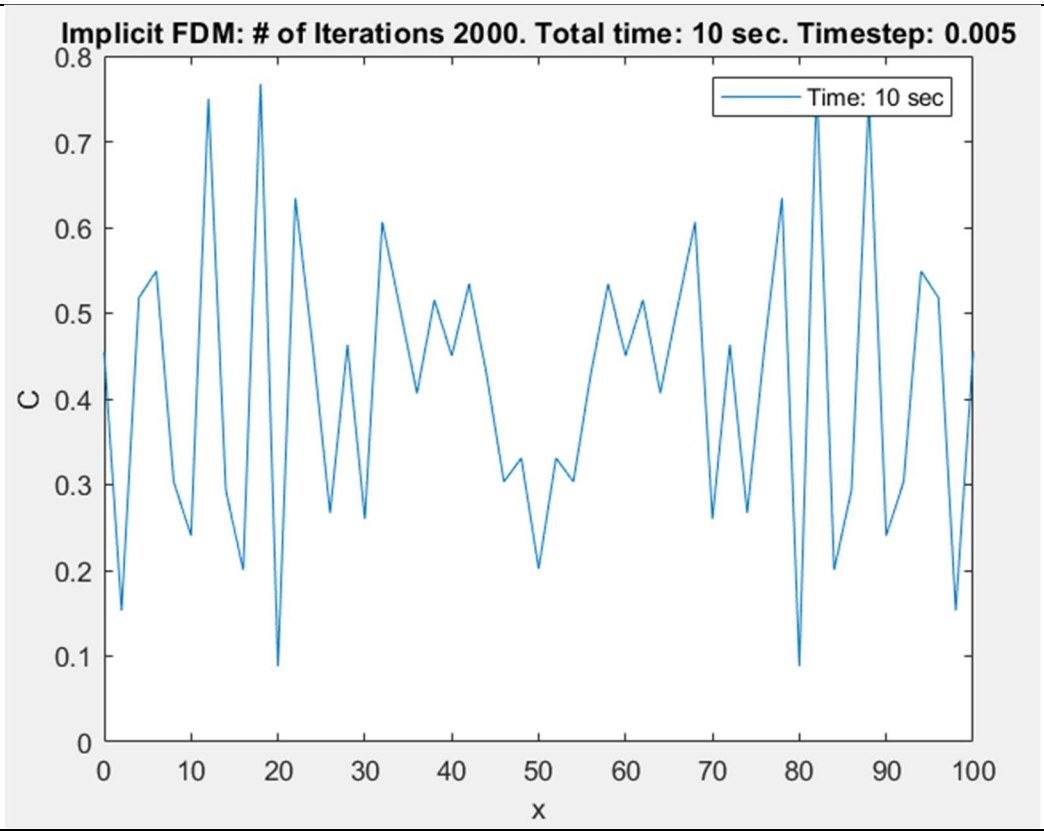

Implicit FDM: # of Iterations 1000. Total time: 5 sec. Timestep: 0.005
Time: 5 sec
C
x


Implicit FDM: # of Iterations 1200. Total time: 6 sec. Timestep: 0.005
Time: 6 sec
C
x

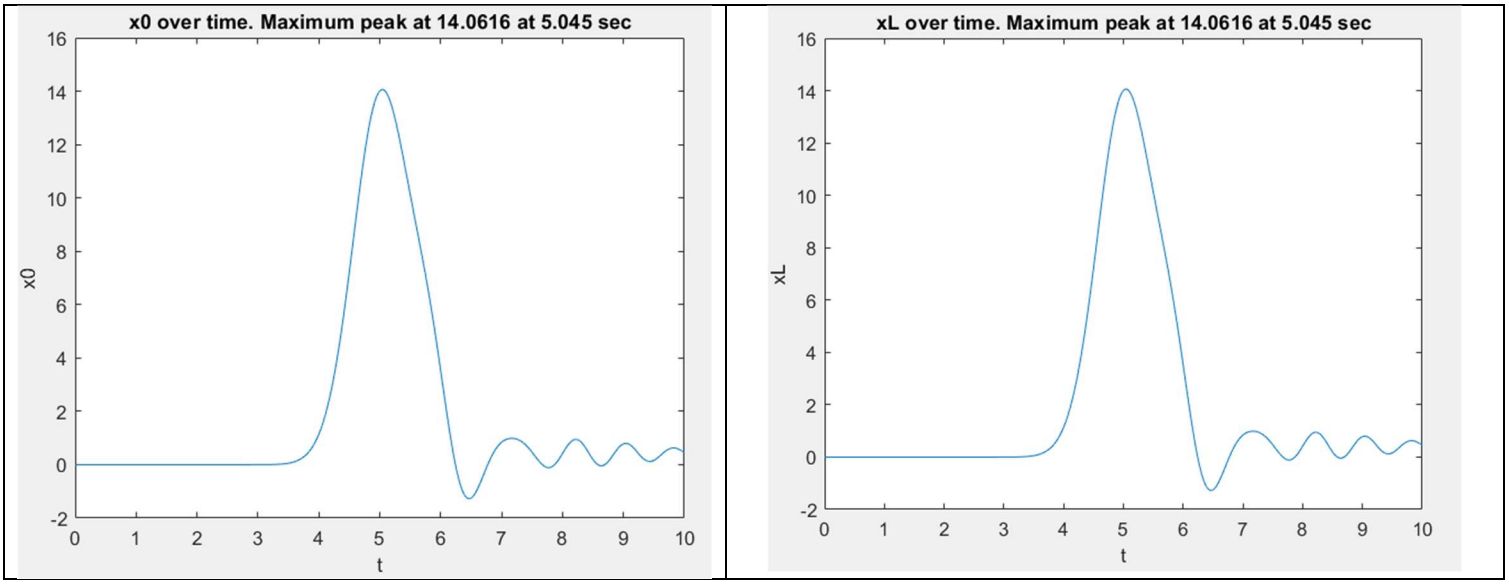

Implicit FDM: # of Iterations 1400. Total time: 7 sec. Timestep: 0.005
Time: 7 sec
C
x


Implicit FDM: # of Iterations 1600. Total time: 8 sec. Timestep: 0.005
Time: 8 sec
C
x


Implicit FDM: # of Iterations 1800. Total time: 9 sec. Timestep: 0.005
Time: 9 sec
C
x



2) Plot the complete time history of your solution at x=0 cm and x=100 cm



c) What are the maximum magnitudes of the wave peaks reaching x=0 cm and x=100 cm? Does the value make sense – why or why not, explain using available information about problem? Also, report the time it takes for the maximum peak of

the action potential to reach the boundary at x=0 cm and x=100 cm, does it make sense – why or why not, explain using the available information about problem?

Answer: Maximum magnitudes for wave peaks reaching x=0 cm and x=100 cm are both *14.016 mv* at *t=5.045 sec* due to the symmetric characteristic of the problem. This makes sense since *t=0* we pump in the potential with magnitude *30mv*, then the profile of our domain almost dissipates at *t=10sec* (from series of figure in b)). Since it is symmetric, we get equal magnitudes on both sides of the boundary, and ~half of *10sec* for the lobes to travel to the edges.

```
%% ---------------- Diffusion - Problem 3-----------------
clear all

r0 = 10; % cm
x0 = 50; % cm;
dx = 2; % cm
h=dx;
Lx = 100; %cm
c = 9.905; % cm/s
tau = 0.05; % sec
x=[0:dx:Lx];
dt = 0.005; %sec
theta = 0.5;

r = sqrt((x-x0).^2);

A = 30 * cos(pi * r / (2*r0) ) ;
A(r>r0) = 0;
A = [0,A,0]; % extend PBC
Aprev = A;
Anext_new = A;
Anext_old = A;
time_step = 0;
time_points = [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10];
tolCheck = 10*eps;
k = c^2*dt^2 / (h^2);

figure(1), clf
plot(x,A(2:end-1),'DisplayName',['Time: '+  string(time_step*dt)+' sec'])
legend(gca,'show')
xlabel('x')
ylabel('C')
title(['Implicit FDM: # of Iterations '+ string(time_step)+ '. Total time: '
+ string(time_step*dt)+ ' sec. ' + 'Timestep: '+ string(dt)]);

x0 = [A(2)];
xL = [A(end-1)];
t = [0];

while (time_step*dt < 10)
    time_step=time_step+1;
    if time_step > 1
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```
        Aprev = A;
        A = Anext_new;
    elseif time_step == 1
        Aprev = A;
        Anext_new = A;
    end
    Anext_old = Anext_new;
    itr=0;
    pitr=0;
    error=1;
    while (error > 1e-5 & itr < 10000)
        i=2;
        Anext_new(i) = -1 / (1 + tau*dt/2 + k*theta + k*h/(c*dt) +
k*theta*tau*h/(2*c)) * ...
            ( ...
            -k*theta* Anext_old(i+1) + ...
            (-2 + ( 2*k + h*k*tau/c)*(1-theta) )* A(i) + (-2*k*(1-
theta))*A(i+1) + ...
            (1 - tau*dt/2 + k*theta - k*h/(c*dt) +
k*theta*h*tau/(2*c))*Aprev(i) + (-k*theta)*Aprev(i+1) ...
            );

        for i=3:(length(A)-2)
            Anext_new(i) =  -1 / (1 + tau*dt/2 + k*theta) * ...
                (...
                (-k*theta/2)*Anext_old(i-1) + (-k*theta/2)*Anext_old(i+1)
+...
                (-k*(1-theta))*A(i-1) + (-2 + 2*k*(1-theta))*A(i) + (-k*(1-
theta))*A(i+1) +...
                (-k*theta/2)*Aprev(i-1) + (1 - tau*dt/2 + k*theta)*Aprev(i)
+ (-k*theta/2)*Aprev(i+1)...
                );
        end

        i=length(A)-1;
        Anext_new(i) = -1 / (1 + tau*dt/2 + k*theta + k*h/(c*dt) +
k*theta*tau*h/(2*c)) * ...
            ( ...
            (-k*theta)* Anext_old(i-1) + ...
            (-2 + ( 2*k + h*k*tau/c)*(1-theta) )* A(i) + (-2*k*(1-
theta))*A(i-1) + ...
            (1 - tau*dt/2 + k*theta - k*h/(c*dt) +
k*theta*h*tau/(2*c))*Aprev(i) + (-k*theta)*Aprev(i-1) ...
            );

         error=max(max(abs(Anext_new-Anext_old)))/max(max(Anext_old));
         itr=itr+1;
         Anext_old = Anext_new;
         pitr=pitr+1;
    end
    % compute shadow nodes
    i=2;
    Anext_new(i-1) = (-2*h/(c*theta*dt)) * ( ...
         (Anext_new(i) - Aprev(i)) ...
```

```
        - c*dt * ( theta/(2*h) * (Anext_new(i+1) + Aprev(i+1) - Aprev(i-1))
+ (1-theta)/h*(A(i+1) - A(i-1)) ) ...
        + tau*dt *(theta*( Anext_new(i) + Aprev(i) )/2 + (1-theta)*A(i))
...
        );

    i=length(A)-1;
    Anext_new(i+1) = (-2*h/(c*dt*theta)) * ( ...
        (Anext_new(i) - Aprev(i)) ...
        + c*dt * (theta/(2*h) * ( -Anext_new(i-1) + Aprev(i+1) - Aprev(i-
1)) + ((1-theta)/h)*(A(i+1) - A(i-1)) ) ...
        + tau*dt *(theta*( Anext_new(i) + Aprev(i) )/2 + (1-theta)*A(i))
...
        );

    t(end+1) = time_step*dt;
    x0(end+1) = Anext_new(2);
    xL(end+1) = Anext_new(end-1);

   % plot
   if any(abs(time_points - time_step*dt) <= tolCheck)
          figure(time_step)
          plot(x,Anext_new(2:end-1), 'DisplayName',['Time: '+
string(time_step*dt)+' sec'])
          legend(gca,'show')
          xlabel('x')
           ylabel('C')
           title(['Implicit FDM: # of Iterations '+ string(time_step)+ '.
Total time: ' + string(time_step*dt)+ ' sec. ' + 'Timestep: '+ string(dt)]);

   end
end


[PkAmp, PkTime] = findpeaks(x0);
[~,idx] = sort(PkAmp,'descend');
max_x0 = PkAmp(idx(1)); %Amplitude of the peak
max_time_x0 = t(PkTime(idx(1))); %Time of the peak

[PkAmp, PkTime] = findpeaks(xL);
[~,idx] = sort(PkAmp,'descend');
max_xL = PkAmp(idx(1)); %Amplitude of the peak
max_time_xL = t(PkTime(idx(1))); %Time of the peak


figure(1)
plot(t,x0)
xlabel('t')
ylabel('x0')
title(['x0 over time. Maximum peak at '+ string(max_x0) + ' at '+
string(max_time_x0) + ' sec']);


figure(2)
plot(t, xL)
```

```
xlabel('t')
ylabel('xL')
title(['xL over time. Maximum peak at '+ string(max_xL)+ ' at '+
string(max_time_xL) + ' sec']);
```