```
%HW-3 Prb-7
%Navneet Singh (nsingh1@andrew.cmu.edu)
function problem7

%The equation was converted to dimensionless form as follows :
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$$\frac{d^2\theta}{d\xi^2} + (\frac{2}{\xi})\frac{d\theta}{d\xi} - \frac{kR^2}{D}\theta = 0$$

$$\frac{d^2\theta}{d\xi^2} + (\frac{2}{\xi})\frac{d\theta}{d\xi} - \phi^2\theta = 0$$

```
clc %clearning screen
clear all %clearing previous stored variables
close all %closing previous plots

%Part (A)
%value of Theile modulus
theile = [0.01, 10];

%running loop to guess intial condition

for i = 1:length(theile)
    thl = theile(i);
    %we know at \xi = 1, \theta = 1. We will make different initial
 guesses
    %for \theta(0) and see whether \theta(\xi=1) is 1 or not.
    %We can make use of fsolve to do this

    %using fsolve to guess initial conditions
    guess = 1; %guess to use fsolve
    theta1 = 1; %given BC and our shooting target
    options = optimset('display','off');
    sol(i) = fsolve(@func, guess,options);

    fprintf('\nFor phi^2 = %f, Initial condition is theta(0) = %f
 ',thl, sol(i));
    fprintf('\nGradient of concentration at outer edge of pellet = %f
\n' ,u(end,2));
    %plotting
    subplot(2,1,i)
    p(i) = plot(t,u(:,1));
    title('Shooting method \theta vs \xi')
    xlabel('\xi');
    ylabel('\theta');
    l = char('\phi^2 = 0.01', '\phi^2 = 10');
    legend(l(i,:))
```

```
end

%Function giving our differential equations
function f = eqn(t, u)
        f = zeros(2,1);
        f(1) = u(2);
        if t == 0
            f(2) = thl*u(1);
        else
            f(2) = thl*u(1) - (2/t)*u(2);
        end
end
%function which checks value of theta(xi=1)
function y = func(guess)
        tspan = [0, 1]; %range of integration
        initial = [guess, 0];  %initial conditions for ode45
        options = odeset('RelTol',1e-5,'AbsTol',[1e-5 1e-5]);
        [t, u] = ode45(@eqn, tspan, initial, options);
        y = theta1 - u(end,1); %checking whether calculated value
 mathches given boundary condition.

end



%Part (B)


%We will disctretize the given differential equation and form system
% as Ax = b. Where x is a vector containing values of theta,

%number of mesh
n = 50;
%distance between two consecutive mesh points, or step size.
h = 1/n;

%step size is to be chosen carefully. If it too small, matrix A or B
 might
%become singular. If it is too large then we will get incorrect
 results.

zy = linspace(0,1,n+1);
%Initializing A and b matrix
A = zeros(n+1,n+1);
b = zeros(n+1,1);
%Different values of Thiele modulus
theil = [0.01, 10];

%running loop for different values of theil modulas
for j = 1:length(theil)

    %Values of p, q and r
    p = -2 ./ (zy);
```

```
    q = theil;
    r = zeros(size(p));

    %Dirichlet BC
    A(n+1, n+1) = 1;
    A(n+1,n) = 0;
    b(n+1) =1;

    %Neumann BC
    A(1,1) = 2 + (h^2)*theil(j);
    A(1,2) = -2;
    b(1) = 0;

    %creating matrix A and b.
    for i = 2:n

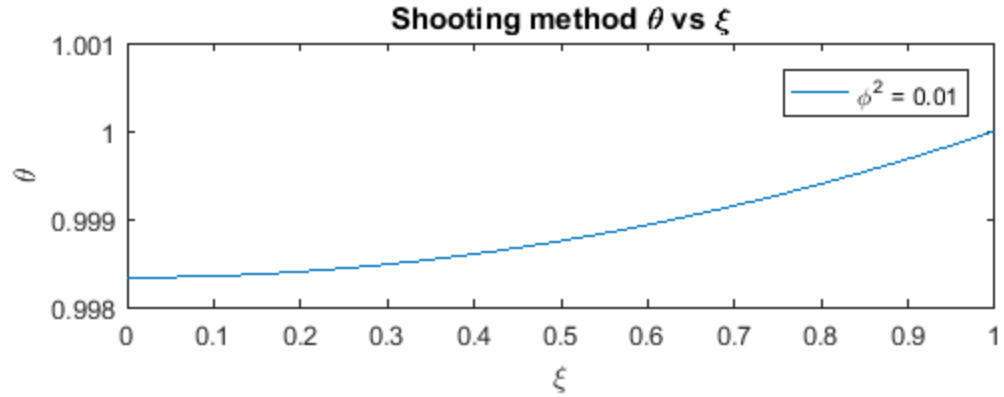
        %calculating values of l,d and u
        d = 2 + (h^2)*theil(j);
        u = -1 + (h/2)*p(i);
        l = -1 - (h/2)*p(i);

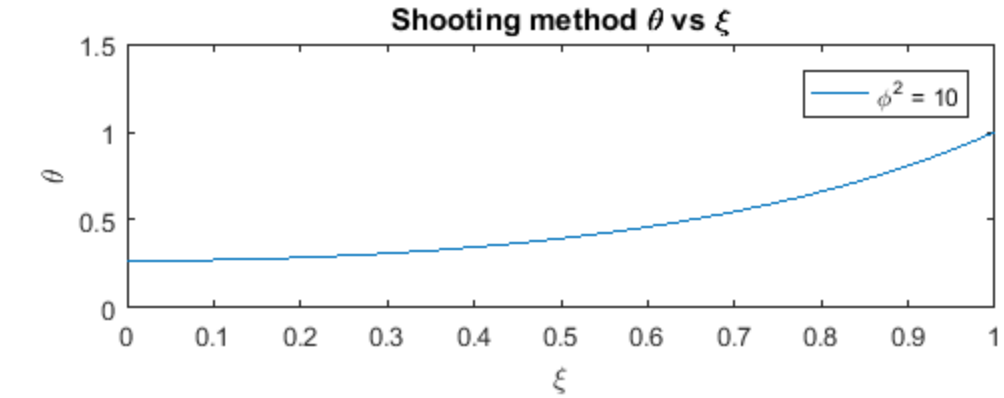
        %matrix A
        A(i, i-1)   = l;
        A(i, i) = d;
        A(i, i+1) = u;
    end
% calculating values of theta
    c(:,j) = A\b;
end

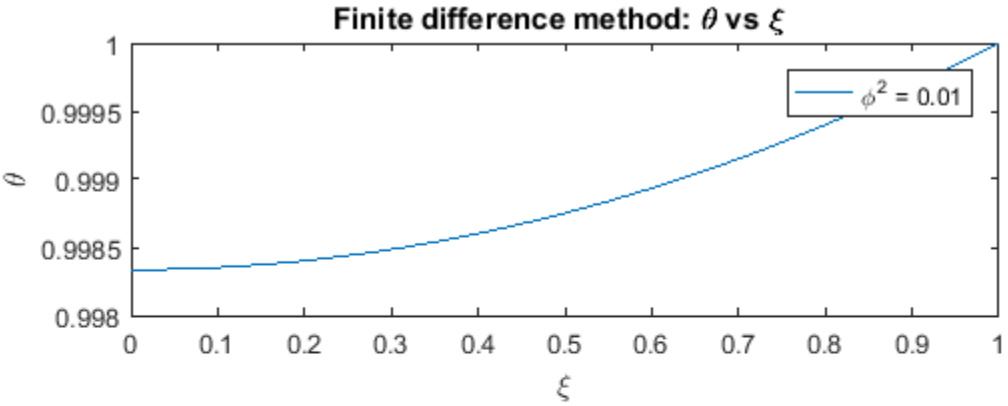
figure
subplot(2,1,1);
plot(zy, c(:,1))
title('Finite difference method: \theta vs \xi ')
xlabel('\xi')
ylabel('\theta')
legend('\phi^2 = 0.01')
subplot(2,1,2);
plot(zy, c(:,2))
xlabel('\xi')
ylabel('\theta')
legend('\phi^2 = 10')
```

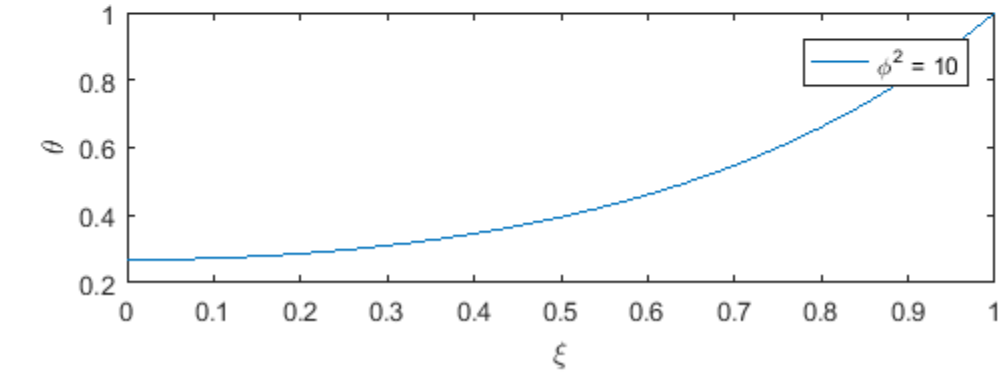
For phi^2 = 0.010000, Initial condition is theta(0) = 0.998335
Gradient of concentration at outer edge of pellet = 0.003331

For phi^2 = 10.000000, Initial condition is theta(0) = 0.268194
Gradient of concentration at outer edge of pellet = 2.173631


Shooting method θ vs ξ
ϕ^2 = 0.01
θ
ξ


Shooting method θ vs ξ
ϕ^2 = 10
θ
ξ


Finite difference method: θ vs ξ
ϕ^2 = 0.01
θ
ξ


ϕ^2 = 10
θ
ξ

```
end
```

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