Benjamin Bemis Numerical Method's HW6 AME 60614

21. Chemical reactions often give rise to stiff systems of coupled rate equations. The time history of a reaction of the following form:

$$A_1 \rightarrow A_2$$
$$A_2 + A_3 \rightarrow A_1 + A_3$$
$$2A_2 \rightarrow 2A_3$$

is governed by the following rate equations

$$\dot{C}_1 = -k_1C_1 + k_2C_2C_3$$
$$\dot{C}_2 = k_1C_1 - k_2C_2C_3 - 2k_3C_2^2$$
$$\dot{C}_3 = 2k_3C_2^2$$

where k_1, k_2, and k_3 are reaction rate constants given as

$$k_1 = 0.04, \quad k_2 = 10.0, \quad k_3 = 1.5 \times 10^3,$$

and the C_i are the concentrations of species A_i. Initially, $C_1(0) = 0.9$, $C_2(0) = 0.1$, and $C_3(0) = 0$.

(a) What is the analytical steady state solution? Note that these equations should conserve mass, that is, $C_1 + C_2 + C_3 = 1$.

(b) Evaluate the eigenvalues of the Jacobian matrix at $t = 0$. Is the problem stiff?

(c) Solve the given system to a steady state solution ($t = 3000$ represents steady state in this problem) using

(i) Fourth-order Runge–Kutta (use (b) to estimate the maximum time step).

(ii) A stiff solver such as *Numerical Recipes*' `stifbs`, `lsode`, or MATLAB's `ode23s`.

Make a log–log plot of the concentrations C_i vs. time. Compare the computer time required for these two methods.

(d) Set up the problem with a linearized trapezoidal method. What advantages would such a scheme have over fourth-order RK?

a.)

$$0 = -k_1C_1 + k_2C_2C_3$$
$$0 = k_1C_1 - k_2C_2C_3 - 2k_3C_2^2$$
$$0 = 2k_3C_2^2$$
$$1 = C_1 + C_2 + C_3$$
$$\boxed{C_1 = C_2 = 0 \quad + \quad C_3 = 1}$$

b.)

$$J = \begin{bmatrix} \frac{\partial \dot{C}_1}{\partial C_1} & \frac{\partial \dot{C}_1}{\partial C_2} & \frac{\partial \dot{C}_1}{\partial C_3} \\ \frac{\partial \dot{C}_2}{\partial C_1} & \frac{\partial \dot{C}_2}{\partial C_2} & \frac{\partial \dot{C}_2}{\partial C_3} \\ \frac{\partial \dot{C}_3}{\partial C_1} & \frac{\partial \dot{C}_3}{\partial C_2} & \frac{\partial \dot{C}_3}{\partial C_3} \end{bmatrix} = \begin{bmatrix} -k_1 & k_2C_3 & k_2C_2 \\ k_1 & -k_2C_3 - 4k_3C_2 & -k_2C_2 \\ 0 & 4k_3C_2 & 0 \end{bmatrix}$$

$$\text{Det}(A - \lambda I) = 0$$

$$\det \begin{bmatrix} -k_1-\lambda & k_2C_3 & k_2C_2 \\ k_1 & -k_2C_3 - 4k_3C_2 - \lambda & -k_2C_2 \\ 0 & 4k_3C_2 & 0\lambda \end{bmatrix}$$

$$\lambda_1 = -598.99 \quad \lambda_2 = 0 \quad \lambda_3 = -1.0417$$

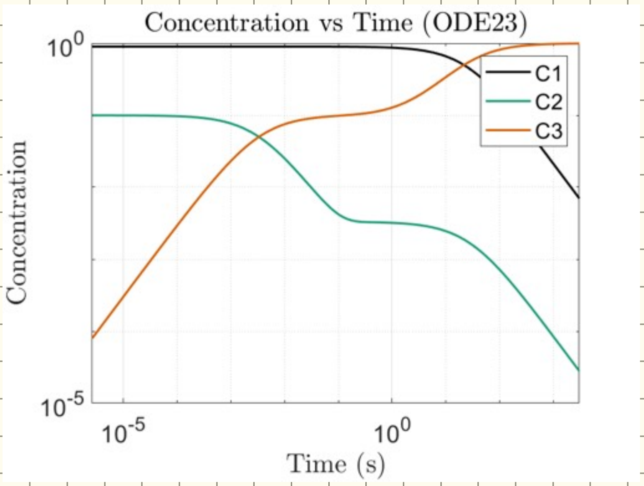
$$\frac{|\lambda|_{max}}{|\lambda|_{min}} \gg 1 \rightarrow \frac{598.99}{1.0417} = 574.99 \quad \text{very stiff}$$

c.) RK4 Stability

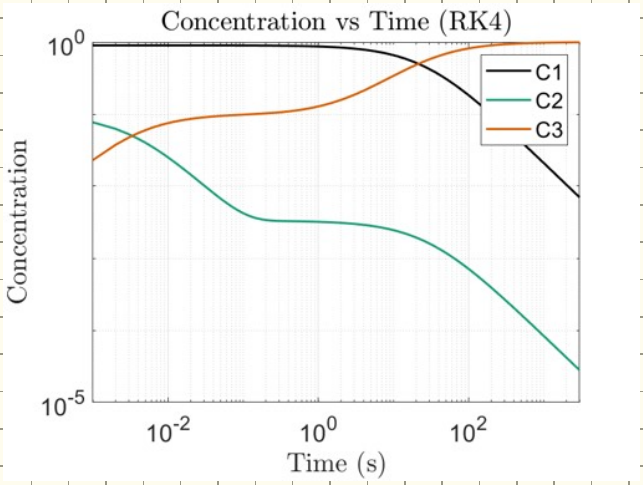
$$\lambda h + \frac{\lambda^2h^2}{2} + \frac{\lambda^3h^3}{6} + \frac{\lambda^4h^4}{24} + 1 \leq 1 \rightarrow \lambda h + \frac{\lambda^2h^2}{2} + \frac{\lambda^3h^3}{6} + \frac{\lambda^4h^4}{24} = 0$$

Solve for h with $\lambda = -599$

$$\boxed{\text{max step size} = 0.0046}$$



Solution time 0.07 s



$h = 0.001$

Solution time 2.33 s

Slight variations are due to the step size In order to solve to the same accuracy substantially more Time is needed.

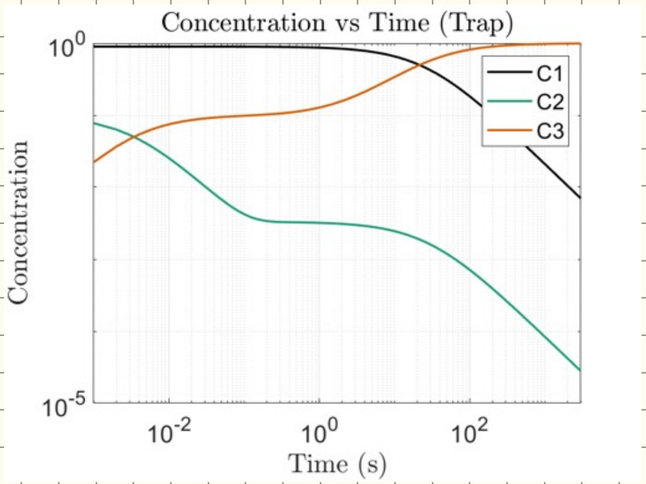
D.) Linearized trapezoidal

$$y_{n+1} = y_n + \frac{h}{2}\left[f(t_n, y_n) + f(t_{n+1}, y_{n+1})\right]$$

$$y^*_{n+1} = y_n + hf(t_n, y_n)$$

$$y_{n+1} = y_n + \frac{h}{2}\left[f(t_n, y_n) + f(t_{n+1}, y^*_{n+1})\right]$$

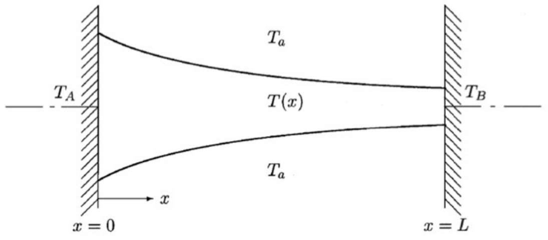
The linearized trapezoidal method is more stable than RK4 and therefore can handle much larger time steps due to its implicit stability. Furthermore it is simplier to calculate and therefore faster.



$h = 0.001$

Solution time 1.78 s

26. The diagram shows a body of conical section fabricated from stainless steel immersed in air at a temperature $T_a = 0$. It is of circular cross section that varies with x. The large end is located at $x = 0$ and is held at temperature $T_A = 5$. The small end is located at $x = L = 2$ and is held at $T_B = 4$.



Conservation of energy can be used to develop a heat balance equation at any cross section of the body. When the body is not insulated along its length and the system is at a steady state, its temperature satisfies the following ODE:

$$\frac{d^2T}{dx^2} + a(x)\frac{dT}{dx} + b(x)T = f(x), \tag{1}$$

where $a(x)$, $b(x)$, and $f(x)$ are functions of the cross-sectional area, heat transfer coefficients, and the heat sinks inside the body. In the present example, they are given by

$$a(x) = -\frac{x+3}{x+1}, \qquad b(x) = \frac{x+3}{(x+1)^2}, \qquad \text{and} \qquad f(x) = 2(x+1) + 3b(x).$$

(a) In this part, we want to solve (1) using the shooting method.

(i) Convert the second-order differential equation (1) to a system of 2 first-order differential equations.

a.)

i.) $T'' + \alpha(x)T' + \beta(x)T = f(x) \rightarrow T'' + \alpha(x)T' + \beta(x)T - f(x) = 0$

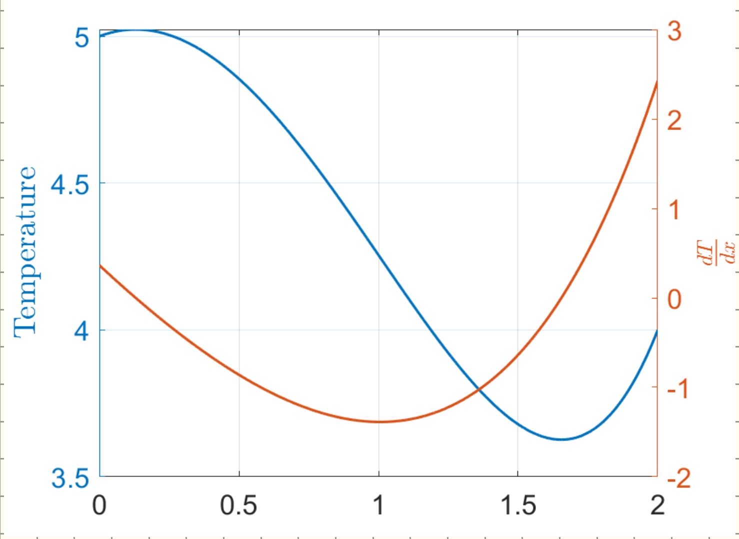
$T_1 = T$

$T_2 = T'$

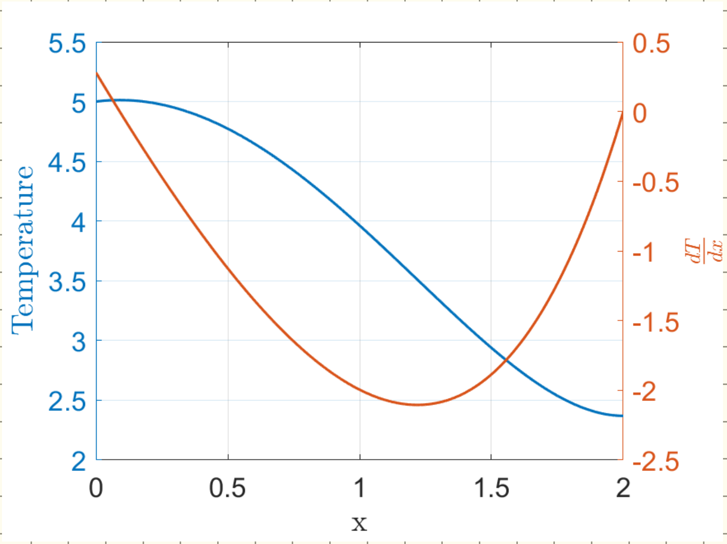
$$\boxed{\begin{aligned} T_1' &= T_2 \\ T_2' &= -\alpha(x)T_2 - \beta(x)T_1 + f(x) \end{aligned}}$$

ii.) $T_L = 4$

iii.) $\frac{dT}{\partial x}\Big|_{x=L} = 0$



x



(b) We now want to solve (1) directly by approximating the derivatives with finite difference approximations. The interval from $x = 0$ to $x = L$ is discretized using N points (including the boundary points):

$$x_j = \frac{j-1}{N-1} L \quad j = 1, 2, \ldots, N.$$

The temperature at point j is denoted by T_j.

(i) Discretize the differential equation (1) using the central difference formulas for the second and first derivatives. The discretized equation is valid for $j = 2, 3, \ldots, N-1$ and therefore yields $N-2$ equations for the unknowns $T_1, T_2, \ldots, T_N$.

(ii) Obtain two additional equations from the boundary conditions ($T_A = 5$ and $T_B = 4$) and write the system of equations in matrix form $AT = f$. Solve this system with $N = 21$. Plot the temperature using symbols on the same plot of part (a)(ii).

i

$$T'' = \frac{T_{j+1} - 2T_j + T_{j-1}}{(\Delta x)^2} \qquad \Delta x = \frac{L}{N-1}$$

$$T' = \frac{T_{j+1} - T_{j-1}}{2\Delta x}$$

$$\boxed{T'' + \alpha(x) T' + \beta(x) T = f(x) \rightarrow \frac{T_{j+1} - 2T_j + T_{j-1}}{(\Delta x)^2} + a(x) \frac{T_{j+1} - T_{j-1}}{2\Delta x} + B(x) T - f(x) = 0}$$

ii

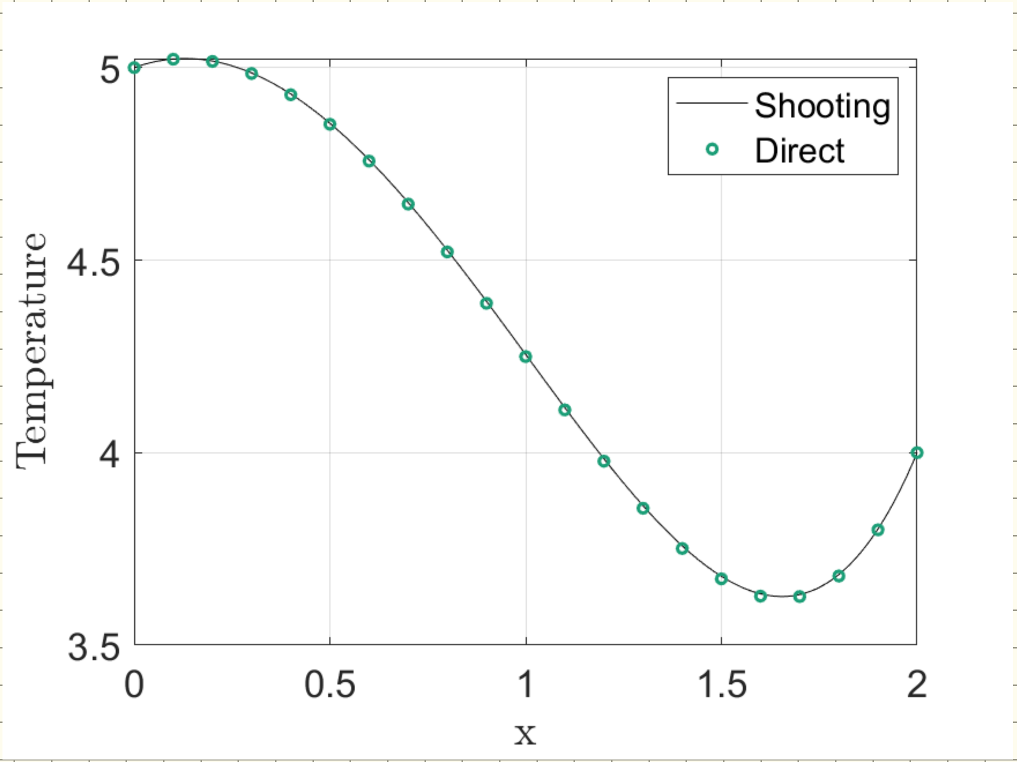
A is $N \times N$

$T_1 = 5$
$T_N = 4$

$AT = f$
$T = A \backslash f$

$$\begin{bmatrix} 1 & & & \\ \frac{1}{dx^2} - \frac{a(x_j)}{2dx} & \frac{-2}{dx^2} + b(x_j) & \frac{1}{dx^2} - \frac{a(x_j)}{2dx} & \\ \ddots & \ddots & \ddots & \\ & & & 1 \end{bmatrix} \begin{bmatrix} T_1 \\ T_j \\ \vdots \\ T_N \end{bmatrix} = \begin{bmatrix} f_1(x_j) \\ f_j(x_j) \\ \vdots \\ f_N(x_j) \end{bmatrix}$$

$f(x_j) = 2(x+1) + 3B(x)$



27. *Mixed boundary conditions.*
With the implementation of boundary conditions in boundary value problems, it is important to preserve the structure of the matrix created by the interior stencil. This often facilitates the solution of the resulting linear equations. Consider the problem in Section 4.11.2 with a mixed boundary condition:

$$ay(0) + by'(0) = g$$

(a) Use the technique suggested in Section 4.11.2 to implement this boundary condition for the problem given by (4.41) and find the new entries in the first row of the matrix.
(b) Alternatively, introduce a ghost point y_{-1} whose value is unknown. Using the equation for the boundary condition and the differential equation evaluated at the point $j = 0$, eliminate y_{-1} to obtain an equation solely in terms of y_0 and y_1. What are the entries in the first row of the matrix?

From 4.41

$$y''(x) + A(x)y'(x) + B(x)y(x) - f(x) = 0$$

$$y(0) = y_0 \qquad y(L) = y_L$$

$$y''(x) = \frac{y_{j+1} - 2y_j + y_{j-1}}{h^2}$$

$$y'(x) = \frac{y_{j+1} - y_{j-1}}{2h}$$

$$\frac{y_{j+1} - 2y_j + y_{j-1}}{h^2} + A(x)\frac{y_{j+1} - y_{j-1}}{2h} + B(x)y(x) = f(x)$$

Rearranging

$$\alpha_j y_{j+1} + \beta_j y_j + \gamma_j y_{j-1} = f_j$$

$$\alpha_j = \left(\frac{1}{h^2} + \frac{A_j}{2h}\right), \quad \beta_j = \left(B_j - \frac{2}{h^2}\right), \quad \gamma_j = \left(\frac{1}{h^2} - \frac{A_j}{2h}\right) \qquad j = 1, 2, 3 \cdots N-1$$

Implimenting B.C.

$$y'(0) \approx \frac{-3y_0 + 4y_1 - y_2}{2h}$$

$$ay(0) + b\left(\frac{-3y_0 + 4y_1 - y_2}{2h}\right) = g$$

$$y(0)\left(a - \frac{3b}{2h}\right) = g - b\frac{4y_1 - y_2}{2h} \rightarrow y(0) = \frac{g - b\frac{4y_1 - y_2}{2h}}{\left(a - \frac{3b}{2h}\right)}$$

$$\alpha_1 y_2 + \beta_1 y_1 = f_1 - \gamma y_0$$

$$\left[\alpha_1 - \frac{\frac{1}{2}b\gamma_1}{a - \frac{3b}{2h}}\right]y_2 + \left[\beta_1 + \frac{\frac{2b}{2h}\gamma_1}{a - \frac{3b}{2h}}\right]y_1 = f_1 - \gamma_1\frac{g}{a - \frac{3b}{2h}}$$

$$A_{1,1} = \alpha_1 - \frac{\frac{1}{2}b\gamma_1}{a - \frac{3b}{2h}} \qquad = f_1 - \gamma_1\frac{g}{a - \frac{3b}{2h}}$$

$$A_{1,2} = \beta_1 + \frac{\frac{2b}{2h}\gamma_1}{a - \frac{3b}{2h}}$$

b.) Using a ghost point

$$y' = \frac{y_{i+1} - y_{i-1}}{2h}$$

$$a y(0) + b\left(\frac{y_1 - y_{-1}}{2h}\right) = g$$

$$y_{-1} = y_1 - \frac{2h}{b}(g - a y_0)$$

$j = 0$

$$y''(0) = \frac{y_1 - 2y_0 + y_{-1}}{h^2} \longrightarrow \frac{y_1 - 2y_0 + y_1 - \frac{2h}{b}(g - a y_0)}{h^2}$$

$$y''(0) = \frac{2(y_1 - y_0)}{h^2} - \frac{2}{bh}(g - a y_0)$$

$$\left(-\frac{2}{h^2} + \frac{2a}{bh}\right) y_0 + \left(\frac{2}{h^2}\right) y_1 + \left(\frac{-2g}{bh}\right) y_2 = f(x)$$

$$\boxed{\begin{aligned} A_{11} &= \left(-\frac{2}{h^2} + \frac{2a}{bh}\right) \\ A_{12} &= \left(\frac{2}{h^2}\right) \\ f_1 &= -\frac{2g}{b\Delta x} \end{aligned}}$$

Contents

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```
%{

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Advisor: Dr Juliano


Description:
AME 60614: Numerical Methods
Homework: 6
Due: 11/22/2024


%}
```

Preperation of the workspace

```
clear all
clc
close all
fontsize = 16;


% set(0,'DefaultFigureWindowStyle','default')
set(0,'DefaultTextInterpreter','latex')
set(0,'DefaultAxesFontSize',fontsize)
set(0,'DefaultLegendFontSize',fontsize)
colors  = ["#000000","#1b9e77","#d95f02","#7570b3","#0099FF"]';
```

Setting data paths

Make sure to update this for the machine that you are working on. (Maybe, This should now run on any machine without change. 7/24/24) Change the current folder to the folder of this m-file.

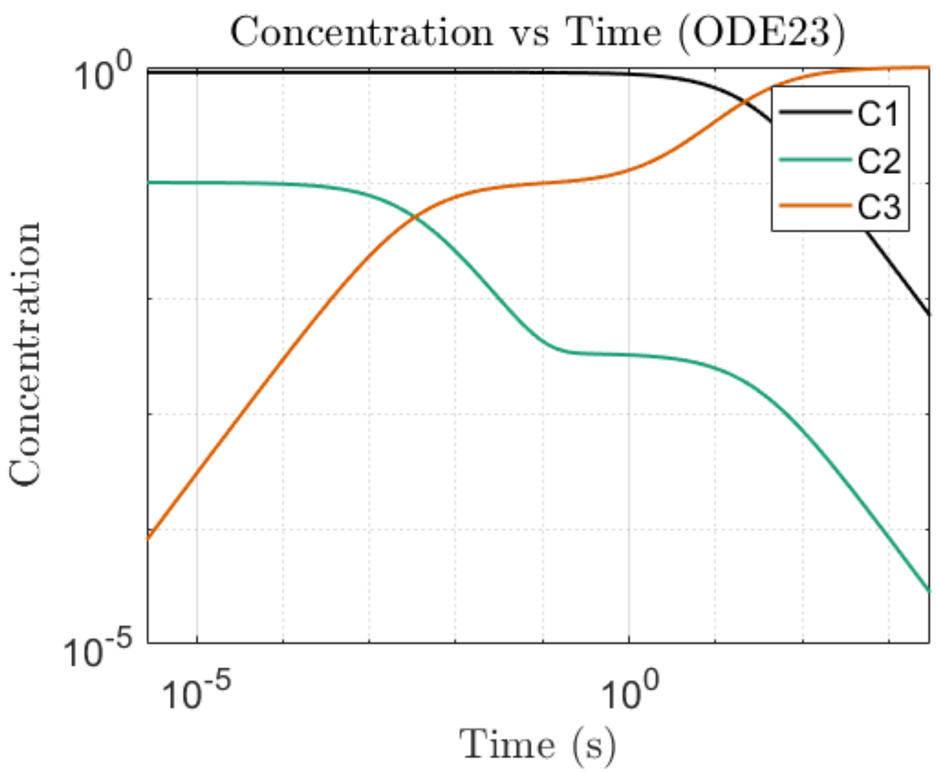
```
if(~isdeployed)
  cd(fileparts(matlab.desktop.editor.getActiveFilename));
end

addpath(cd)
% cd ..; % Moving up a directory (from processing_code)
basepath = cd; % Pulling the current directory


imagepath = [basepath filesep 'images' filesep];
mkdir(imagepath);
```

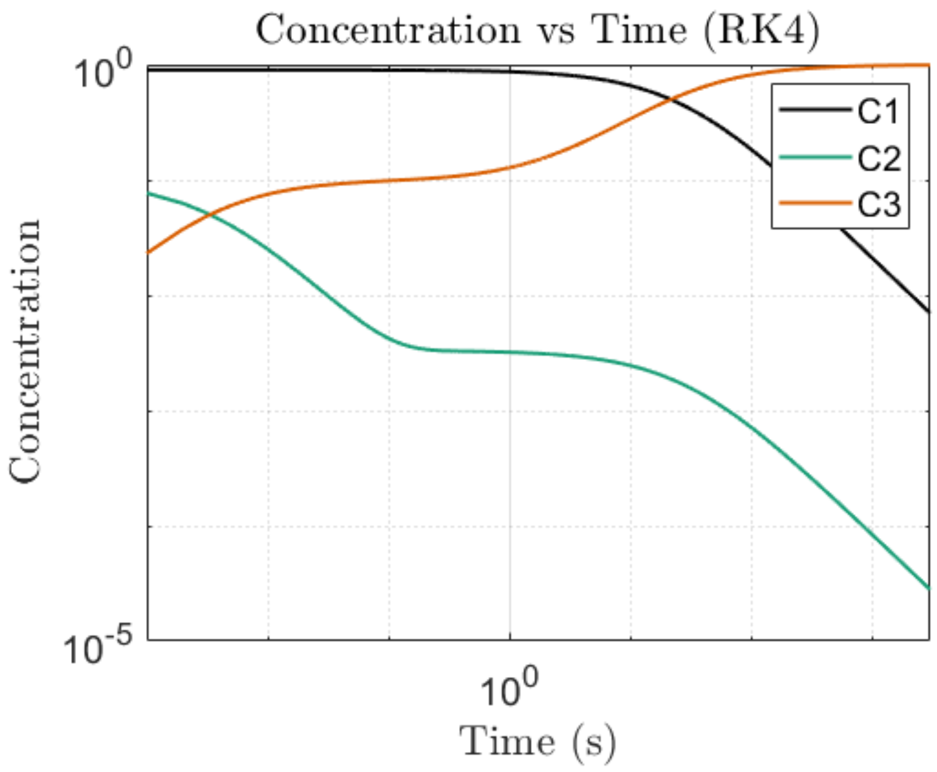
```
Warning: Directory already exists.
```

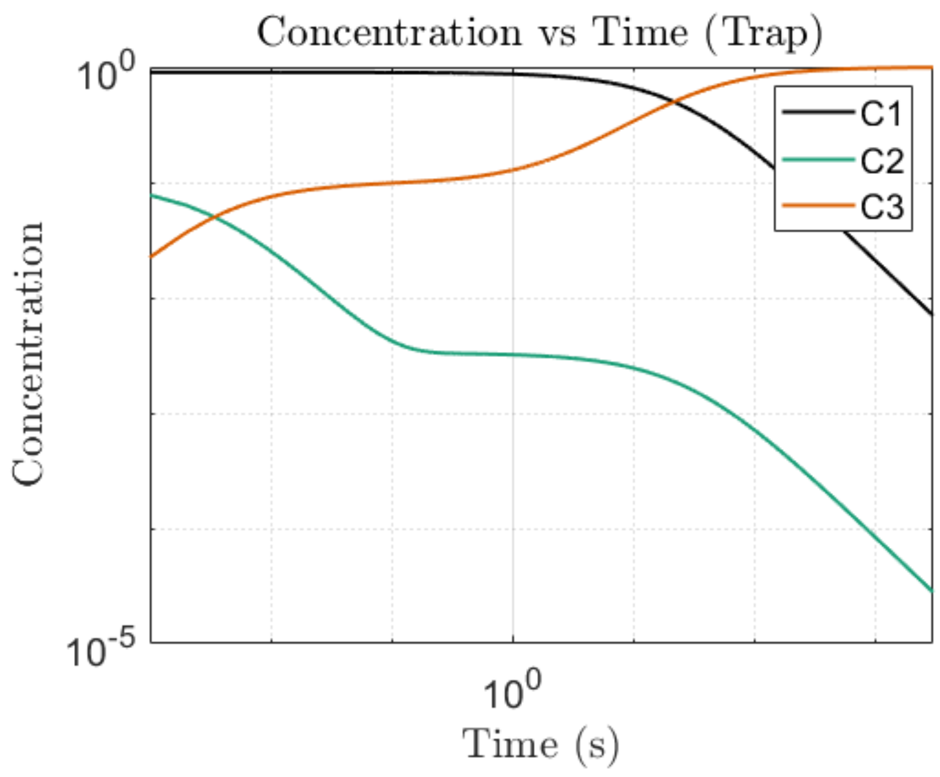
Problem 21 Chapter 4

```
tol = 1e-6;


c1_0 = 0.9;
c2_0 = 0.1;
c3_0 = 0;

k1 = 0.04;
k2 = 10;
k3 = 1.5e3;

A = [-k1 k2*c3_0 k2*c2_0;
    k1 -k2*c3_0-4*k3*c2_0 -k2*c2_0;
    0 4*k3*c2_0 0];

lambda = eig(A);


stiffness = lambda(1)/lambda(3);

% Time span
tspan = [0 3000];

% Initial conditions
C0 = [0.9; 0.1; 0];

stab = @(h) lambda(1)*h + (lambda(1)^2*h^2)/2 +(lambda(1)^3*h^3)/6+(lambda(1)^4*h^4)/24 ;
[root,err] = Nraph(stab,0.01,tol)

% Define the system of ODEs


% Solve using ode23s (stiff solver)
options = odeset('RelTol', 1e-6, 'AbsTol', 1e-9);
tic
[t_stiff, C_stiff] = ode23s(@reaction_rates, tspan, C0, options);
toc

tic
[t_RK, C_RK] = RK4(@reaction_rates, C0, 0, 3000, 1e-3);
toc

tic
[t_trap, C_trap] = trapezoidal_s(@reaction_rates, C0, 0, 3000, 1e-3);
toc

% Plotting the results
figure;
loglog(t_stiff, C_stiff(:,1), '-', 'LineWidth', 1.5, 'Color', colors(1), 'DisplayName', 'C1');
hold on;
loglog(t_stiff, C_stiff(:,2), '-','LineWidth', 1.5, 'Color', colors(2), 'DisplayName', 'C2');
hold on
loglog(t_stiff, C_stiff(:,3), '-','LineWidth', 1.5, 'Color', colors(3), 'DisplayName', 'C3');
xlabel('Time (s)');
ylabel('Concentration');
legend;
```

```
xlim(tspan)
title('Concentration vs Time (ODE23)');
grid on;
print(gcf,[imagepath,'Q23_ode23.png'],'-dpng');



figure;
loglog(t_RK, C_RK(1,:), '-','LineWidth', 1.5, 'Color', colors(1), 'DisplayName', 'C1');
hold on;
loglog(t_RK, C_RK(2,:), '-','LineWidth', 1.5, 'Color', colors(2), 'DisplayName', 'C2');
hold on
loglog(t_RK, C_RK(3,:), '-','LineWidth', 1.5, 'Color', colors(3), 'DisplayName', 'C3');
xlabel('Time (s)');
ylabel('Concentration');
legend;
title('Concentration vs Time (RK4)');
xlim(tspan)
grid on;
print(gcf,[imagepath,'Q23_RK4.png'],'-dpng');


figure;
loglog(t_trap, C_trap(1,:), '-','LineWidth', 1.5, 'Color', colors(1), 'DisplayName', 'C1');
hold on;
loglog(t_trap, C_trap(2,:), '-','LineWidth', 1.5, 'Color', colors(2), 'DisplayName', 'C2');
hold on
loglog(t_trap, C_trap(3,:), '-','LineWidth', 1.5, 'Color', colors(3), 'DisplayName', 'C3');
xlabel('Time (s)');
ylabel('Concentration');
legend;
title('Concentration vs Time (Trap)');
xlim(tspan)
grid on;
print(gcf,[imagepath,'Q23_trap.png'],'-dpng');
```


Concentration vs Time (ODE23)
C1
C2
C3
10^0
10^{-5}
10^{-5}
10^0
Concentration
Time (s)

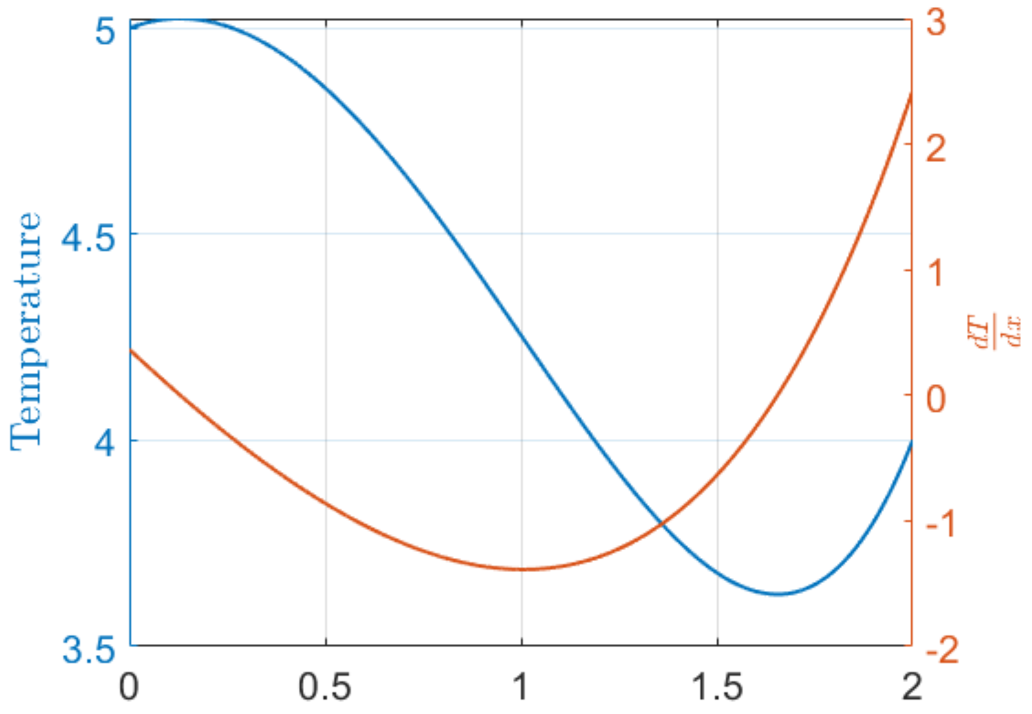

Concentration vs Time (RK4)
C1
C2
C3
10^0
10^{-5}
10^0
Concentration
Time (s)

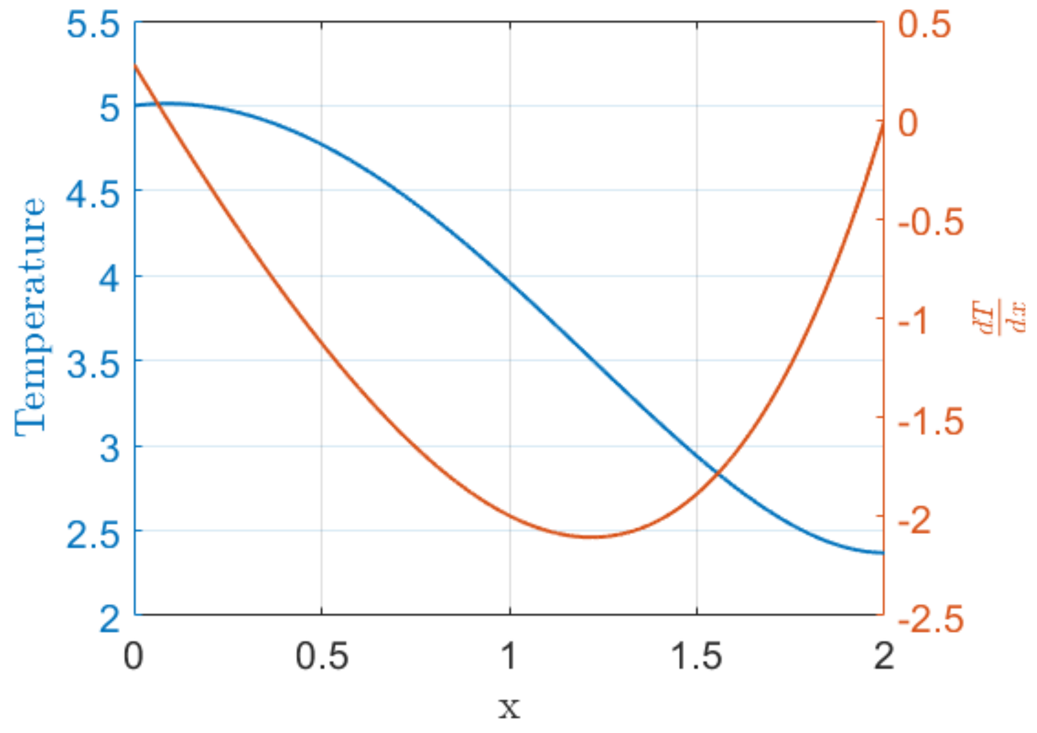


Problem 26 Chapter 4: part a

```
tol = 1e-6;
Ta = 0;
T0 = 5;
TL = 4;
xL = 2;
x_init = 0;
xRange = [x_init xL];
BC = [T0, TL];
h = 0.001;


alpha = @(x) -(x+3)/(x+1);
beta = @(x) (x+3)/(x+1).^2;
f = @(x) 2*(x+1) + 3*beta(x);
f_temp = @(x,T,Tp) -alpha(x)*Tp -beta(x)*T +f(x);

[x_a, y, yp] = shoot(f_temp,xRange,BC , h, -.01 ,tol);

figure
yyaxis left
plot(x_a,y,'LineWidth', 1.5)
hold on
ylabel('Temperature');

yyaxis right
plot(x_a,yp,'LineWidth', 1.5)
xlim(xRange)
ylabel('$\frac{dT}{dx}$');
grid on
print(gcf,[imagepath,'Q26_shoot.png'],'-dpng');

% % testing against ode 45
% f_van = @(x,T,Tp) (1-T^2)*Tp-T;
% [xt, yt, ytp] = shoot(f_van,[0 20],[2,2] , h, -.01 ,tol);
%
% figure
% yyaxis left
% plot(xt,yt)
% hold on
% yyaxis right
% plot(xt,ytp)


% part a) iii.

[x, ydf, ypdf] = shootdf(f_temp,xRange,[5,0] , h, -.01 ,tol);
figure
yyaxis left
plot(x,ydf, 'LineWidth', 1.5)
hold on
ylabel('Temperature');
yyaxis right
plot(x,ypdf, 'LineWidth', 1.5)
xlim(xRange)
grid on
xlabel('x');
ylabel('$\frac{dT}{dx}$');
print(gcf,[imagepath,'Q26_shoot2.png'],'-dpng');
```

```
    "counter = "    "1"


err =

    7.1917

    "counter = "    "2"


err =

    2.3919


err =

   7.9492e-14


ans =

    0.3652

    "counter = "    "1"


err =

    8.2856

    "counter = "    "2"


err =
    5.9925


err =

   2.4919e-13


ans =

    0.2801
```

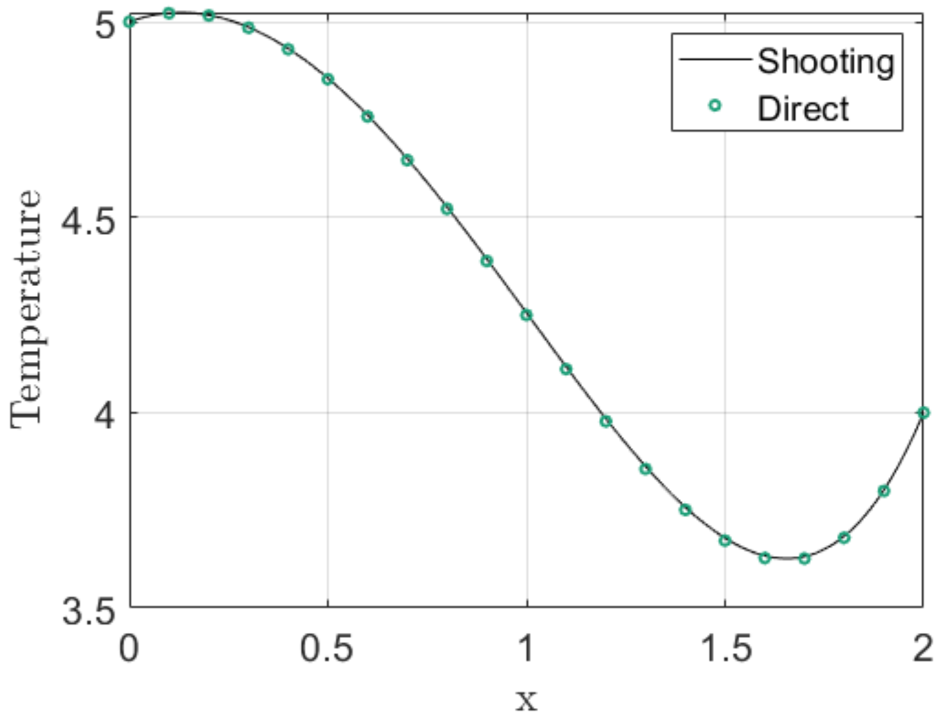




Problem 26 Chapter 4: part b

```
L = 2;
N = 21;                 % Number of points
x = linspace(0, L, N); % Discretized grid points
dx = L / (N-1);         % Grid spacing
T_A = 5;                % Boundary condition at x = 0
T_B = 4;                % Boundary condition at x = L

% Initialize A matrix and f vector
A = zeros(N, N);
f_vec = zeros(N, 1);

% Set boundary conditions in f vector
f_vec(1) = T_A;
f_vec(N) = T_B;

% Fill the A matrix and f vector
for j = 2:N-1
    xj = x(j);
    a_j = alpha(xj);
    b_j = beta(xj);
    f_j = f(xj);

    % Coefficients for T_{j-1}, T_j, T_{j+1}
    A(j, j-1) = 1 / dx^2 - a_j / (2 * dx);
    A(j, j)   = -2 / dx^2 + b_j;
    A(j, j+1) = 1 / dx^2 + a_j / (2 * dx);

    % Right-hand side value
    f_vec(j) = f_j;
end

% Boundary conditions
A(1,1) = 1;
```

```
A(N,N) = 1;

% Solve the system AT = f
T = A \ f_vec;

% Plotting the results
figure;
plot(x_a,y,'k')
hold on
plot(x, T, 'o', 'MarkerSize', 4, 'LineWidth', 1.5, Color=colors(2));
xlabel('x');
ylabel('Temperature');
% title('Temperature Distribution using Finite Difference');
grid on;
legend('Shooting',"Direct");
print(gcf,[imagepath,'Q26_direct.png'],'-dpng');
```



Problem 27 Chapter 4

Functions

```
function [root,err] = Nraph(f,initGuess,tol)
%Nraph solves for the root nearest the initial guess using the Newt-Raphson
%method.

% INPUTS:
% f: is a function handle.
% initGuess: is the inital guess for the root.
% tol: desired tolerance.

% OUTPUTS:
% root: nearest root to initial guess.
% err: error in the solution of the root.

x = initGuess;
```

```
x(2) = initGuess+1;
counter = 2;
while abs(f(x(end))) >= tol

x(counter+1) = x(counter) - f(x(counter)) * (x(counter)-x(counter-1))/(f(x(counter))-f(x(counter-1)));

counter = counter+1;
end
root = x(counter);
err =  abs(f(root));

end

function [x, y1, y2] = shoot(f,xRange, BC, h, dx_guess ,tol)

% x = xRange(1):h:xRange(2);

dx = dx_guess;
dx(2) = dx_guess+.5;

%
y1 = inf;
% [x, y1, y2] = RK4_2(f, BC(1), dx_guess, xRange(1), xRange(2), h);

counter = 1;
while abs(y1(end)- BC(2)) >= tol

    if counter == 1
        [x, y1, y2] = RK4_2(f, BC(1), dx_guess, xRange(1), xRange(2), h);
        disp(["counter = ", string(counter)])

    elseif counter == 2
        [x, y1, y2] = RK4_2(f, BC(1), dx_guess+.5, xRange(1), xRange(2), h);
        disp(["counter = ", string(counter)])
         dx(counter+1) = dx(counter) - (y1(end)-BC(2)) * (dx(counter) - dx(counter-1))/ (y1(end)-y_prev(counter));
    elseif counter > 2
        [x, y1, y2] = RK4_2(f, BC(1), dx(counter), xRange(1), xRange(2), h);
        dx(counter+1) = dx(counter) - (y1(end)-BC(2)) * (dx(counter) - dx(counter-1))/ (y1(end)-y_prev(counter));

    end

y_prev(counter+1) = y1(end);
err = abs(y1(end)- BC(2))
counter = counter+1;
end
dx(end-1)
end

function [x, y1, y2] = shootdf(f,xRange, BC, h, dx_guess ,tol)

% x = xRange(1):h:xRange(2);

dx = dx_guess;
dx(2) = dx_guess+.5;

%
y2 = inf;
% [x, y1, y2] = RK4_2(f, BC(1), dx_guess, xRange(1), xRange(2), h);

counter = 1;
while abs(y2(end)- BC(2)) >= tol
```

```
    if counter == 1
        [x, y1, y2] = RK4_2(f, BC(1), dx_guess, xRange(1), xRange(2), h);
        disp(["counter = ", string(counter)])

    elseif counter == 2
        [x, y1, y2] = RK4_2(f, BC(1), dx_guess+.5, xRange(1), xRange(2), h);
        disp(["counter = ", string(counter)])
         dx(counter+1) = dx(counter) - (y2(end)-BC(2)) * (dx(counter) - dx(counter-1))/ (y2(end)-y_prev(counter));
    elseif counter > 2
        [x, y1, y2] = RK4_2(f, BC(1), dx(counter), xRange(1), xRange(2), h);
        dx(counter+1) = dx(counter) - (y2(end)-BC(2)) * (dx(counter) - dx(counter-1))/ (y2(end)-y_prev(counter));

    end

y_prev(counter+1) = y2(end);
err = abs(y2(end)- BC(2))
counter = counter+1;
end
dx(end-1)
end

function dCdt = reaction_rates(t, C)
k1 = 0.04;
k2 = 10;
k3 = 1.5e3;

% Unpack concentrations
C1 = C(1);
C2 = C(2);
C3 = C(3);

% System of differential equations
dC1 = -k1 * C1 + k2 * C2 * C3;
dC2 = k1 * C1 - k2 * C2 * C3 - 2 * k3 * C2^2;
dC3 = 2 * k3 * C2^2;

% Return as a column vector
dCdt = [dC1; dC2; dC3];
end

function [t, y1, y2] = RK4_2(f, y0, v0, t0, tf, h)

    % RK4_2 works for single equation odes

    % Inputs:
    %   f  - Function handle for y'' = f(t, y, y')
    %   y0 - Initial condition for y (y(t0) = y0)
    %   v0 - Initial condition for y' (y'(t0) = v0)
    %   t0 - Initial time
    %   tf - Final time
    %   h  - Step size
    %
    % Outputs:
    %   t  - Array of time steps
    %   y1 - Array of solution values for y at each time step
    %   y2 - Array of solution values for y' at each time step

    % Define the time vector from t0 to tf with step size h
    t = t0:h:tf;
    N = length(t); % Number of time steps
    y1 = zeros(1, N); % Preallocate y1 for y
    y2 = zeros(1, N); % Preallocate y2 for y'
```

```matlab
    % Set the initial conditions
    y1(1) = y0;
    y2(1) = v0;

    % Apply the 4th-order Runge-Kutta method
    for n = 1:N-1
        % Calculate k1 values
        k1_y1 = y2(n);
        k1_y2 = f(t(n), y1(n), y2(n));

        % Calculate k2 values
        k2_y1 = y2(n) + h/2 * k1_y2;
        k2_y2 = f(t(n) + h/2, y1(n) + h/2 * k1_y1, y2(n) + h/2 * k1_y2);

        % Calculate k3 values
        k3_y1 = y2(n) + h/2 * k2_y2;
        k3_y2 = f(t(n) + h/2, y1(n) + h/2 * k2_y1, y2(n) + h/2 * k2_y2);

        % Calculate k4 values
        k4_y1 = y2(n) + h * k3_y2;
        k4_y2 = f(t(n) + h, y1(n) + h * k3_y1, y2(n) + h * k3_y2);

        % Update y1 and y2 using weighted average of slopes
        y1(n+1) = y1(n) + (h/6) * (k1_y1 + 2*k2_y1 + 2*k3_y1 + k4_y1);
        y2(n+1) = y2(n) + (h/6) * (k1_y2 + 2*k2_y2 + 2*k3_y2 + k4_y2);
    end
end

function [t, Y] = RK4(f, Y0, t0, tf, h)
    % RK4 - 4th-order Runge-Kutta method for systems of equations.
    %
    % Inputs:
    %   f  - Function handle for the system of equations, f(t, Y)
    %        Y is a column vector, and f should return a column vector.
    %   Y0 - Initial conditions as a column vector (Nx1, where N is the number of equations)
    %   t0 - Initial time
    %   tf - Final time
    %   h  - Step size
    %
    % Outputs:
    %   t  - Array of time steps
    %   Y  - Solution matrix (NxM, where N is the number of equations, M is the number of time steps)

    % Define the time vector from t0 to tf with step size h
    t = t0:h:tf;
    N = length(t);       % Number of time steps
    num_eqns = length(Y0);  % Number of equations in the system

    % Preallocate the solution matrix Y
    Y = zeros(num_eqns, N);

    % Set the initial conditions
    Y(:, 1) = Y0;

    % Apply the 4th-order Runge-Kutta method for each time step
    for n = 1:N-1
        % Calculate k1 values
        k1 = f(t(n), Y(:, n));

        % Calculate k2 values
        k2 = f(t(n) + h/2, Y(:, n) + h/2 * k1);
        % Calculate k3 values
        k3 = f(t(n) + h/2, Y(:, n) + h/2 * k2);

        % Calculate k4 values
        k4 = f(t(n) + h, Y(:, n) + h * k3);

        % Update Y using the weighted average of slopes
        Y(:, n+1) = Y(:, n) + (h/6) * (k1 + 2*k2 + 2*k3 + k4);
    end
end

function [t, Y] = trapezoidal_s(f, Y0, t0, tf, h)
    % trapezoidal_s - Linearized Trapezoidal method for systems of ODEs.
    %
    % Inputs:
    %   f  - Function handle for the system of equations, f(t, Y)
    %        Y is a column vector, and f should return a column vector.
    %   Y0 - Initial conditions as a column vector (Nx1, where N is the number of equations)
    %   t0 - Initial time
    %   tf - Final time
    %   h  - Step size
    %
    % Outputs:
    %   t  - Array of time steps
    %   Y  - Solution matrix (NxM, where N is the number of equations, M is the number of time steps)

    % Define the time vector from t0 to tf with step size h
    t = t0:h:tf;
    N = length(t);       % Number of time steps
    num_eqns = length(Y0);  % Number of equations in the system

    % Preallocate the solution matrix Y
    Y = zeros(num_eqns, N);

    % Set the initial conditions
    Y(:, 1) = Y0;

    % Apply the Linearized Trapezoidal method for each time step
    for n = 1:N-1
        % Predictor step (Euler's method)
        Y_star = Y(:, n) + h * f(t(n), Y(:, n));

        % Corrector step
        Y(:, n+1) = Y(:, n) + (h/2) * (f(t(n), Y(:, n)) + f(t(n+1), Y_star));
    end
end
```

```
root =

    0.0046


err =

   8.8988e-08

Elapsed time is 0.073169 seconds.
Elapsed time is 2.258758 seconds.
Elapsed time is 1.849003 seconds.
```