## Contents



```
%{

@author: Benjamin Bemis Ph.D Student,
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.

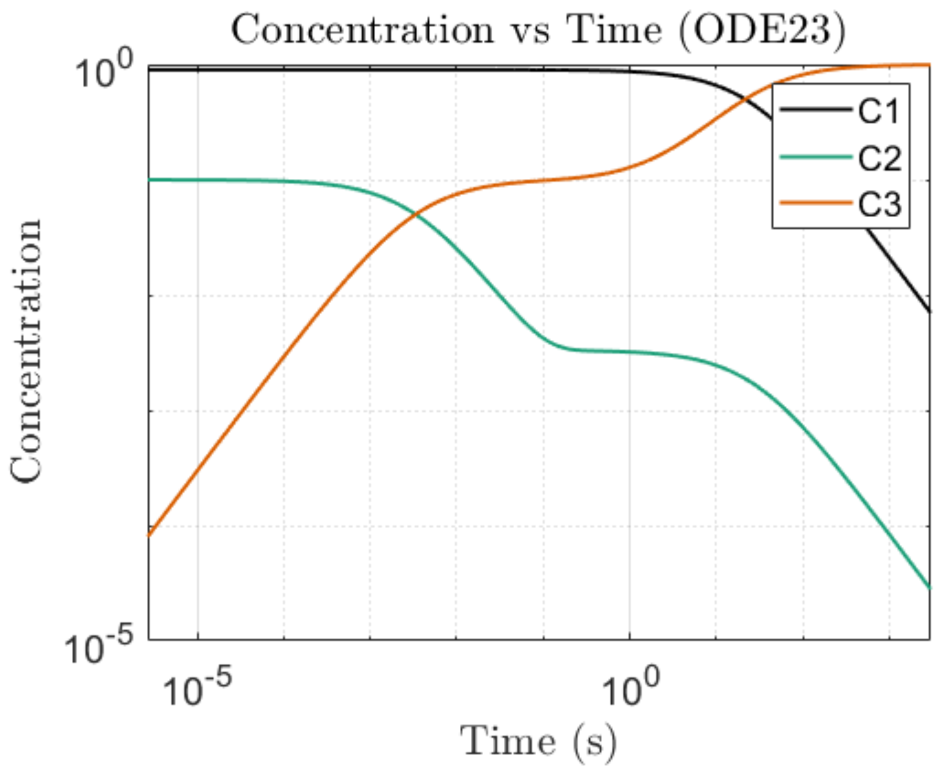
```
if(~isdeployed)
  cd(fileparts(matlab.desktop.editor.getActiveFilename));
end

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


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

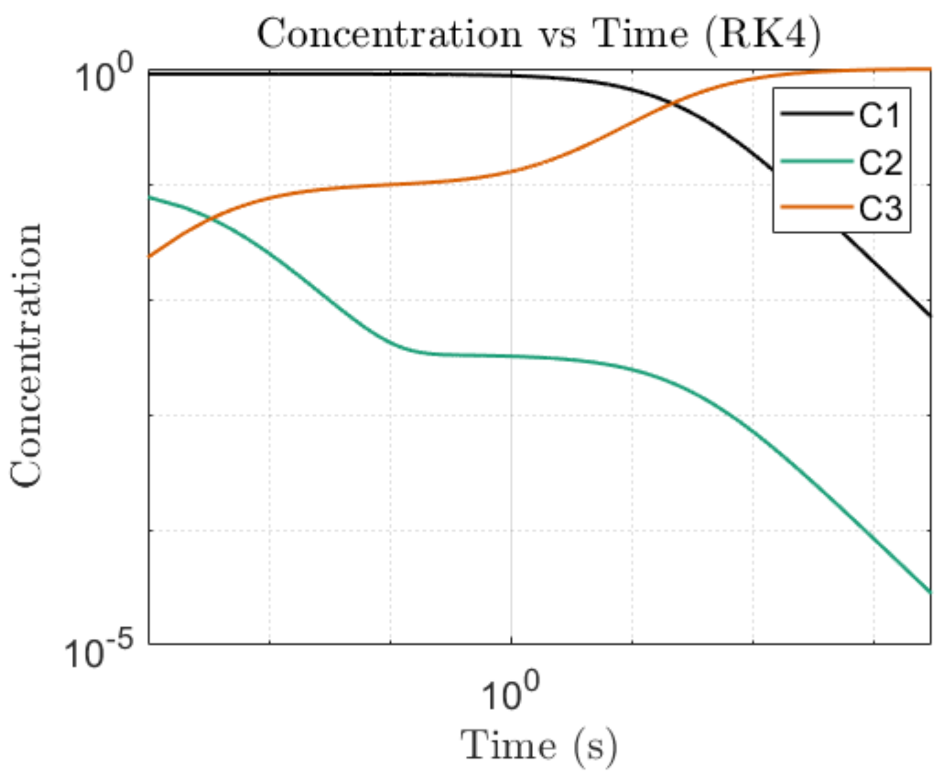
```
Warning: Directory already exists.
```

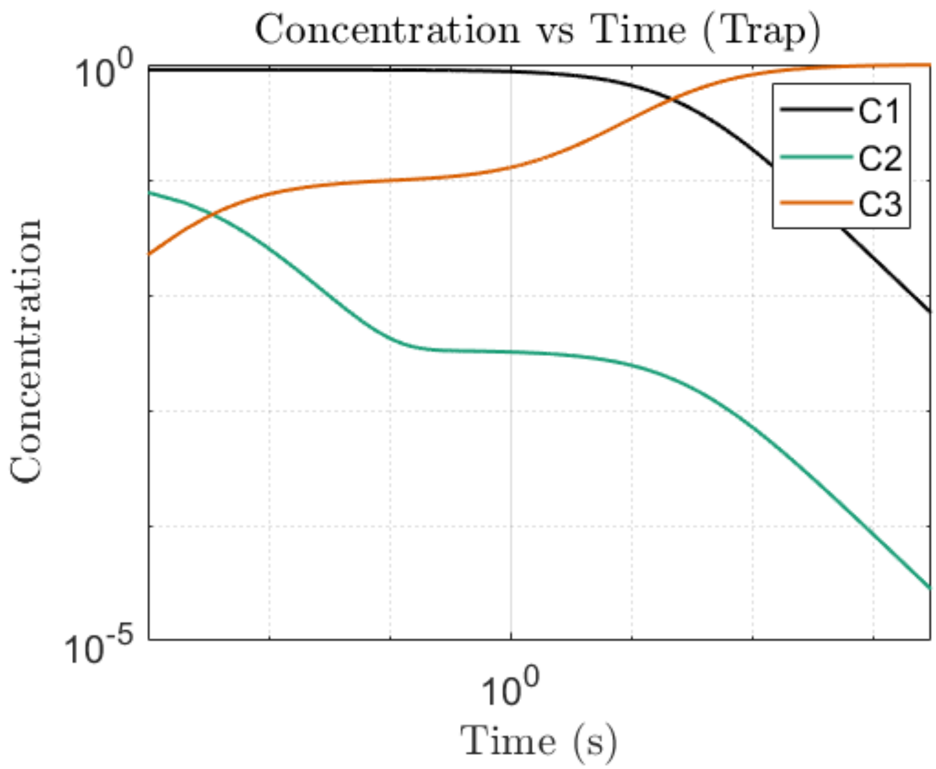
### Problem 21 Chapter 4

```
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)
$10^0$
$10^{-5}$
Concentration
$10^{-5}$
$10^0$
Time (s)
C1
C2
C3


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



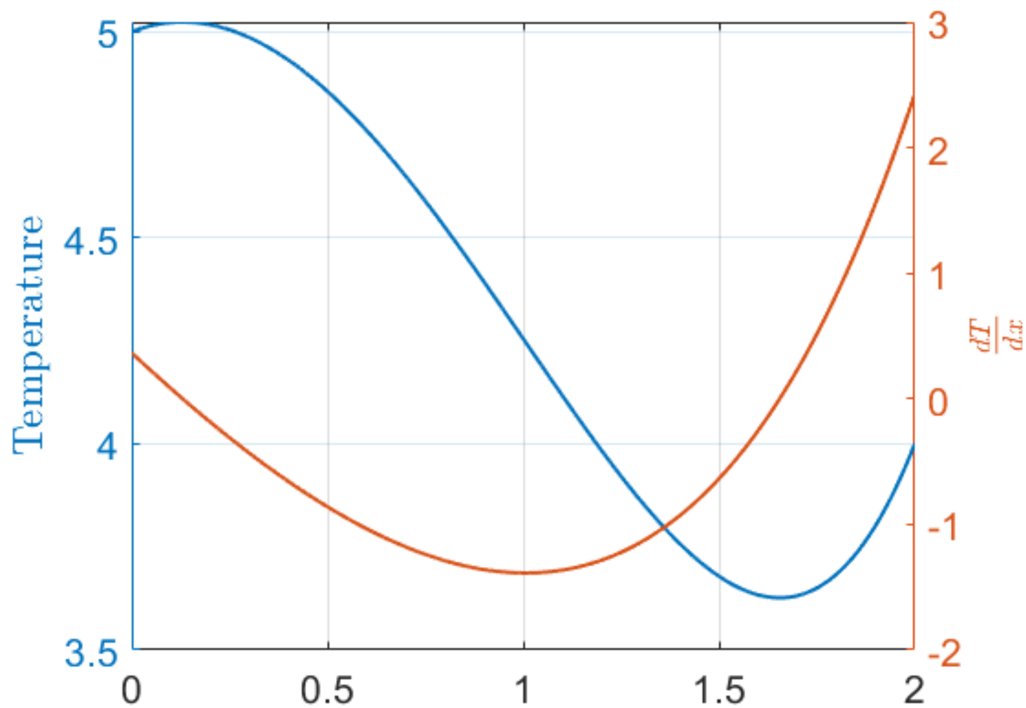

### Problem 26 Chapter 4: part a

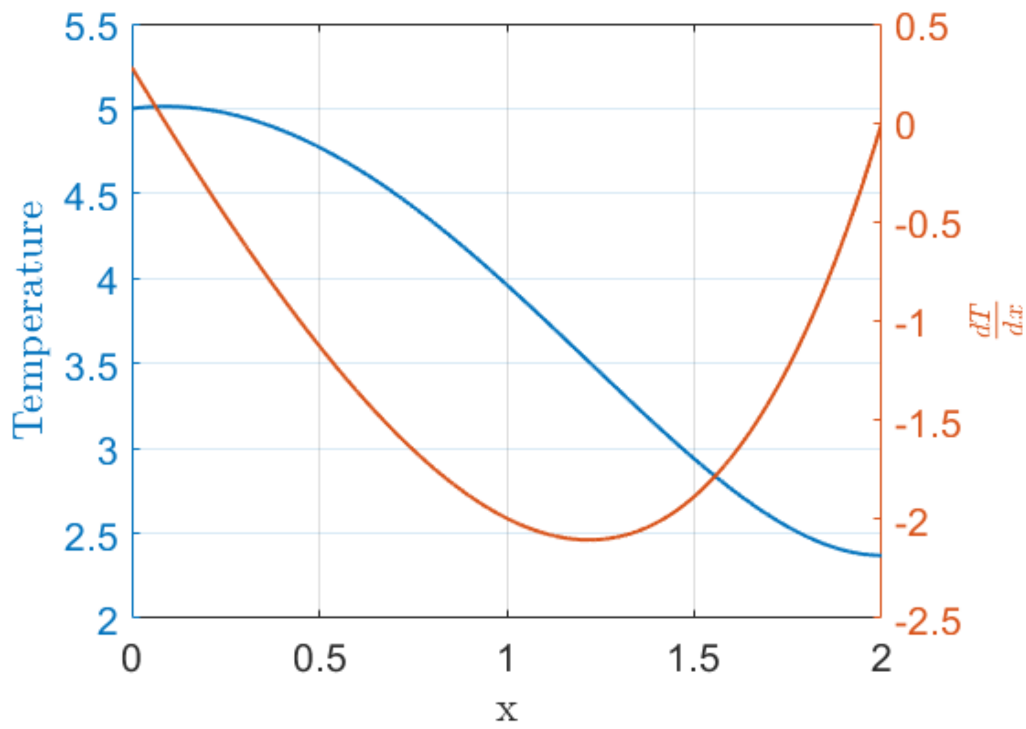
```
tol = 1e-6;
Ta = 0;
T0 = 5;
TL = 4;
xL = 2;
x_init = 0;
xRange = [x_init xL];
BC = [T0, TL];
h = 0.001;


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
```

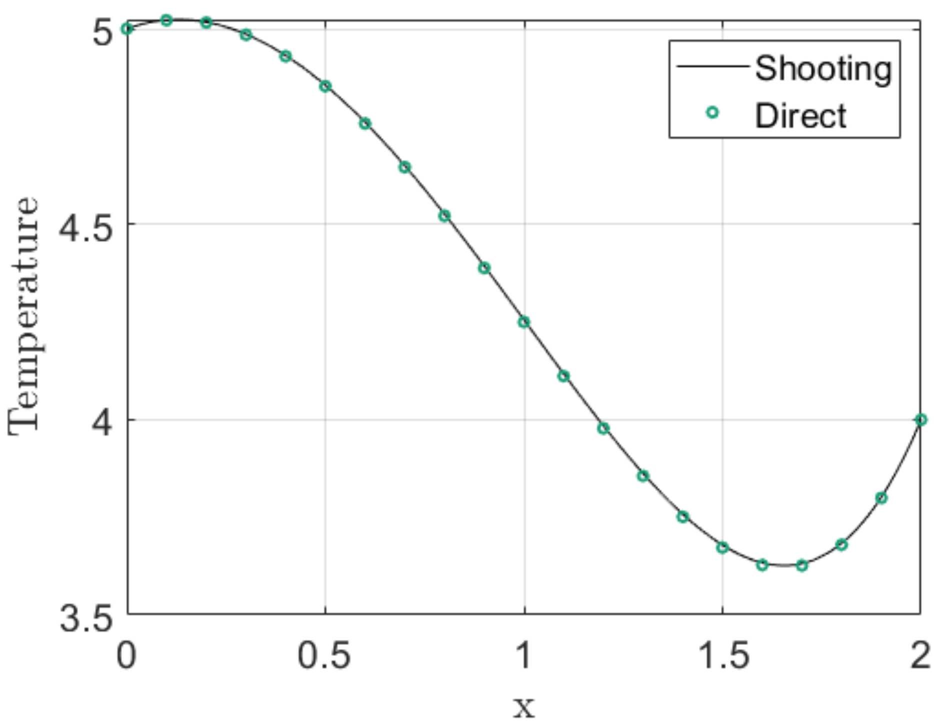





### Problem 26 Chapter 4: part b

```
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.
```