Homework Assignment Number Three

Problem (1)

Consider the initial value problem:

$$\frac{dy}{dx} + a(x)y = b(x)$$

where we have an initial condition of the form:

$$y(x = x_o) = y_o$$

with the specific values given by:

$$a(x) = 2 , \qquad b(x) = x\sin(3x) , \;\; y(x = 0) = 1$$

(a) Analytically solve for y(x) from x = 0 to 4.
(b) Plot the analytical solution.
(c) Use Euler with a time step of 0.4
(d) Use Euler with a time step of 0.04
(e) Use Runge-Kutta with a time step of 0.4
(f) Use Runge-Kutta with a time step of 0.04
(g) Compare the relative error of the Euler estimate of y(x=4) for both sized steps. Explain.
(h) Compare the relative error of the Runge-Kutta estimate of y(x=4) for both sized steps. Explain.
(i) Compare the relative errors of the Euler and Runge-Kutta estimates of y(x=4) for a time step of 0.04. Explain.
(j) Compare the relative errors of the Runge-Kutta estimates of y(x=2) and y(x=4) for a time step of 0.04. Explain.

Problem (2)

Numerically solve the acetylene vibrational/translational problem for the initial conditions:

$$\underline{x}(t=0) = \begin{bmatrix} -0.1 \\ 0 \\ 0.25 \\ 0.5 \end{bmatrix} \text{ and initial velocities } \;\; \underline{\dot{x}}(t=0) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

for t = 0 to 2 sec, using the following values for the masses and the spring constants.

$$m_H = 1.0 , \qquad m_C = 12.0 , \qquad k_{HC} = 1.0 , \qquad k_{CC} = 10.0$$

Problem (3)
Find an application from your own experience or a classical problem in your own field of research that results in a system of at least 2 ODEs, linear or nonlinear.

(a) Describe the physical problem from which the equation arises. Describe it in sufficient detail that an engineer from a different discipline could understand it.

(b) Write the ODEs. Write a complete set of reasonable initial conditions.

(c) If possible, analytically solve for the solution(s).

(d) Plot the solution (analytical or numerical).

(e) Explain the physical significance of the solution(s) and its behavior.

Problem (4)
Perform a stability analysis on the linear ODE model you created in Problem (3).

(a) Find the eigenvalues and eigenvectors.

(b) Describe the type of critical point.

(c) Describe the stability of the critical point.

(d) Give a physical description of the eigenvectors.

(e) Show a phase plot with the critical point, eigenvectors, and a couple representative trajectories plotted on it.

Problem (5)
In the notes on ODE stability, there is the example of a first order reaction occurring in an adiabatic CSTR. Repeat the problem when the reaction is second order. Use all of the same parameters as are used in the example in the notes, except make the reactor volume 10 liters.

For those students who are not chemical engineers, I give the parameters and ODEs below. For those students who are chemical engineers, you should be able to derive these ODEs.

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   x = y(1);            % extent of reaction
   T = y(2);            % Temperature K
   Cin = 3.0;           % inlet concentration mol/l
   C = Cin*(1-x);       % concentration
   Q = 60e-3;           % volumetric flowrate l/s
   R = 8.314;           % gas constant J/mol/K
   Ea = 62800;          % activation energy J/mol
   ko = 4.48e+6;        % reaction rate prefactor 1/s
   k = ko*exp(-Ea/(R*T)); % reaction rate constant 1/s
   V = 10;              % reactor volume l
   Cp = 4.19e3;         % heat capacity J/kg/K
   Tin = 298;           % inlet feed temperature K
   Tref = 298;          % thermodynamic reference temperature K
   DHr = -2.09e5;       % heat of rxn J/mol
   rho = 1.0;           % density kg/l
   dydt(1) = 1/V*(Q*Cin - Q*C - k*C*C*V);  % mass balance mol/s
   dydt(2) = 1/(Cp*rho*V)*(Q*Cp*rho*Tin  - Q*Cp*rho*T -
DHr*k*C*C*V);           % NRG balance J/s
   dydt(1) = -1/Cin*dydt(1); % convert conc. to extent
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(a) Find the critical points.

(b) Determine the type and stability of the critical point by plotting a few trajectories in the phase plane.