MAE 290B. Homework 2

Winter 2019

Due Thursday, Feb. 7, in class

Note: *You are expected to provide legible and clear solutions for the homework. Otherwise points will be deducted. Computer programs must be* **written on your own** *and submitted through TritonEd. Plots and sketches must be labeled and the axis well defined. Staple the document and number the pages. Torn-out pages are not allowed.*

1. Consider the following nonlinear ordinary differential equation

$$y' = \frac{\sin(y)}{y} + t^2 \quad , \quad y(0) = 1 \; . \tag{1}$$

a) Explain what is the main disadvantage of integrating Eq.(1) with an implicit scheme.

b) Derive a linearized version of Crank-Nicolson that solves the nonlinear o.d.e, $y' = f(y, t)$. Show that this modification, when applied to the linear equation, $y' = \lambda y$, does not affect the unconditional stability properties of the original method.

c) Describe in detail how to solve Eq.(1) using linearized Crank-Nicolson.

2. A set of chemical reactions during food digestion in the human body is considered. Biological catalysts and enzymes participate in these reactions in such a way that an enzyme A combines with a substance B to form a complex D. The D complex has two possible fates. It can dissociate to B and A or it can proceed to produce P.

$$A + B \underset{k_2}{\overset{k_1}{\rightleftarrows}} D \xrightarrow{k_3} A + P \tag{2}$$

The dynamics of these reactions are described by the following system of non-linear ordinary differential equations:

$$\begin{aligned}
\dot{C}_B &= -k_1 C_B C_A + k_2 C_D \\
\dot{C}_A &= -k_1 C_B C_A + (k_2 + k_3) C_D \\
\dot{C}_D &= k_1 C_B C_A - (k_2 + k_3) C_D \\
\dot{C}_P &= k_3 C_D \; ,
\end{aligned} \tag{3}$$

where every k is a reaction rate constant and $C_i = [i]$ is the concentration of the chemical species.

The initial values of the concentrations are $C_{B0} = 0.5$, $C_{A0} = 7.5 \times 10^{-5}$, $C_{D0} = C_{P0} = 0$ and the reaction rate constants are $k_1 = 2.1 \times 10^3$, $k_2 = 5 \times 10^{-3}$ and $k_3 = 18$.

a) In order to analyze the stability of the system linearize the right hand side to obtain the Jacobian matrix. Look at the eigenvalues at $t = 0$. Is the system stiff?

b) Obtain the time evolution of C_i until steady state using Matlab's function `ode23s`.

c) Implement RK4 to obtain the solution.

d) Using RK4 how would you use theory to obtain the maximum possible time step at each iteration?

3. A body of conical section fabricated from stainless steel is 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:

$$\frac{d^2T}{dx^2} + a(x)\frac{dT}{dx} + b(x)T = f(x), \tag{4}$$

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

$$a(x) = \frac{x+3}{x+1}\,, \qquad b(x) = \frac{x+3}{(x+1)^2}\,, \qquad f(x) = 2(x+1) + 3b(x)\,. \tag{5}$$

a) In this part, we want to solve Eq.4 using the shooting method.

1. Convert the second-order differential equation Eq.4 to a system of 2 first-order differential equations.
2. Use the shooting method to solve the system in 1. Plot the temperature distribution along the body.
3. If the body is insulated at the $x = L$ end, the boundary condition becomes $dT/dx = 0$. In this case use the shooting method to find $T(x)$ and in particular the temperature at $x = L$. Plot the temperature distribution along the body.

b) We now want to solve Eq.4 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):

$$x_j = \frac{j-1}{N-1}L \quad j = 1, 2, \ldots N \tag{6}$$

The temperature at point j is denoted by T_j.

1. Discretize the differential equation Eq.4 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 $T_1, T_2, \ldots, T_N$.
2. 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 using your own implementation of the Thomas algorithm with $N = 21$. Plot the temperature using symbols on the same plot of part a2.