MAE 290B. Homework 2

Winter 2018

Due Thursday, Feb. 8, in class

Note: *You are expected to provide legible and clear solutions for the homework. Otherwise points will be deducted. 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

$$y' = e^{\sin(y)} + ty \quad , \quad y(0) = 1 \ . \tag{1}$$

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.

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

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 $C_{B0} = 0.8$, $C_{A0} = 7.5 \times 10^{-5}$, $C_{D0} = C_{P0} = 0$ and the reaction rate constants are $k_1 = 1.8 \times 10^3$, $k_2 = 1.8 \times 10^{-3}$ and $k_3 = 22$.

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. The equations of fluid motion can be simplified using scaling arguments and self-similarity to describe the flow over a flat plate with a single equation, the well-known Blasius Boundary Layer equation, and boundary conditions. The boundary value problem (BVP) is

$$y''' + yy'' = 0 \quad ; \quad y'(0) = y(0) = 0 \; , y'(\infty) = 1 \; . \tag{4}$$

In order to integrate Eq.(4) we first assume that solutions converge in a finite domain $0 \leq \eta \leq 10$. Then, we convert our third-order problem into a system of three first-order equations by defining $y_1 = y''$, $y_2 = y'$ and $y_3 = y$. This change of variables will give

$$\frac{d\mathbf{y}}{d\eta} = f(\mathbf{y}) \; , \tag{5}$$

where $\mathbf{y} \triangleq [y_1 \;\; y_2 \;\; y_3]'$ is a column vector.

- The given BVP has boundary conditions specified at $y = 0$ and $y = \infty$. Use a shooting method to solve this BVP as if it was an initial value problem (IVP). Implement RK4 to advance the IVP in space and iterate the initial condition using a secant method. Use $y_1^1(0) = 1$ and $y_1^2(0) = 0$ as the initial two guesses to start the secant method.
- Plot $\mathbf{y}(\eta)$ in $0 \leq \eta \leq 6$.
- Plot the evolution of $y_1^\alpha(0)$ with every iteration until at least $|\varepsilon| \triangleq |y_2^\alpha(10) - 1| < 1 \times 10^{-4}$.