Homework # 3

ME526/NSE526

Due: November 3

1. You are encouraged to work in a group of up to 2 students and submit one solution per student.
2. Your solution must be clearly legible. Illegible work may not be graded and returned without any points. Although not necessary, you may type your work.
3. All problems must be solved. However, all problems may not be graded. A random sample of problems will be selected for grading.
4. If you are required to write a computer program, attach your code with several comment statements on the code wherever possible.

1. Consider the following family of implicit methods for the initial value problem $y' = f(y)$,

$$y_{n+1} = y_n + h\left[\theta f(y_{n+1}) + (1-\theta) f(y_n)\right], \tag{1}$$

where $0 \leq \theta \leq 1$ is a parameter. Perform linear stability analysis and plot the stability diagrams for $\theta = 0$, $\theta = 1/4$, $\theta = 3/4$ on the same graph. Compare the schemes and their stability for potentially different types of $f(y)$, i.e. different values of λ for the model problem. Comment on your findings.

For $\theta = 3/4$, discuss if the scheme can be used for a problem where the exact solutions grow unbounded (i.e. $\lambda_R > 0$). Clearly indicate on your diagram what region corresponds to this *growing* solutions.

2. The following scheme has been proposed for solving $y' = f(y)$:

$$y_{n+1} = y_n + \omega_1 k_1 + \omega_2 k_2, \tag{2}$$

where

$$\begin{aligned} k_1 &= h f(y_n) && (3)\\ k_0 &= h f(y_n + \beta_0 k_1) && (4)\\ k_2 &= h f(y_n + \beta_1 k_0) && (5) \end{aligned}$$

with h being the time step.

   (a) Determine the coefficients ω_1, ω_2, β_0 and β_1 that would maximize the order of accuracy of the method. Use Taylor series expansions for k_0, k_1, k_2 etc. to determine the coefficient values. Can you name this scheme?

   (b) Apply this method to $y' = \alpha y$. What is the maximum step size h for α being a purely imaginary number?

   (c) Apply this method to $y' = \alpha y$. What is the maximum step size h for α being a real and negative number?

   (d) Create and draw a stability diagram for this scheme in the $(h\lambda_R, h\lambda_I)$ plane with the method applied to a model problem $y' = \lambda y$.

3. Consider chemical reactions in a reactor:

$$\begin{aligned} A_1 &\rightarrow A_2 && (6)\\ A_2 + A_3 &\rightarrow A_1 + A_3 && (7)\\ 2A_2 &\rightarrow 2A_3 && (8) \end{aligned}$$

The above reaction are governed by the following rate equations:

$$\begin{aligned} \frac{dC_1}{dt} &= -k_1 C_1 + k_2 C_2 C_3 && (9)\\ \frac{dC_2}{dt} &= k_1 C_1 - k_2 C_2 C_3 - 2k_3 C_2^2 && (10)\\ \frac{dC_3}{dt} &= 2k_3 C_2^2 && (11) \end{aligned}$$

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

$$k_1 = 0.04; \quad k_2 = 10.0; \quad k_3 = 1.5 \times 10^3 \tag{12}$$

and C_i are the concentrations of species A_i. Initially, $C_1(0) = 0.9$, $C_2(0) = 0.1$, and $C_3(0) = 0$. Note that at any instant in time $C_1 + C_2 + C_3 = 1$ from conservation of mass.

(a) Find the steady state solution (analytically).

(b) Is the system stiff? Show all steps.

(c) Solve the above system numerically to steady state solution (say $t = 3000$ represents steady state) using

i. RK4. Do you think $\Delta t = 0.003$ will give you a stable solution? Justify your answer based on Stability Analysis at $t = 0$. Use this time-step to obtain the steady state solution. Note the computing time required to obtain steady state (i.e seconds, mins, hours?). Compare steady state solution to the exact. Plot all concentrations on the same plot (use axes ranges from 10^{-5} to 2×10^0 for concentrations and 10^{-5} to 4000 for time. Note the computing time required to obtain steady state (i.e seconds, mins, hours?).

ii. Use a stiff ode solver such as MATLAB's ode23s to get the solution[1]. How many iterations are needed to reach steady state? Plot concentration versus time just as before. Note the computing time required to obtain steady state.
Make a log-log plot of the concentrations versus time (on the same plot). Compare the computer time required for these two methods.

4. Setup the above problem with a **linearized** central differencing (trapezoidal) scheme. Write the system of equations assuming that you are advancing from time level t_n to t_{n+1}.

(a) To do this, first write down the finite-difference equations for the standard Central Differencing scheme. Since this is an implicit method, you will have non-linear terms for the unknown concentrations at time level t_{n+1}. Apply the linearization technique to the unknown non-linear terms in your finite-difference approximation (fda) and re-write the fda indicating the time level at which each term is evaluated. Your final answer should be in the form: $\mathbf{C}\overline{Y} = \mathbf{D}\overline{X} + \overline{b}$ where $\mathbf{C}$, $\mathbf{D}$ are matrices, $\overline{Y}$, $\overline{X}$, and $\overline{b}$ are some vectors. Clearly indicate the elements of each matrix and vector and also the time level at which each element is evaluated.

(b) What advantages would such a linearized central differencing scheme have over say the fourth-order RK method? Do you think a time step of say five times larger than the time step used in the above part (i.e. $\Delta t = 0.015$) would give a stable solution? If it does, solve the system of equations using this linearized central differencing scheme and this time step. Compare the computing time required to obtain the steady state solution. Also compare your solution to the solution obtained in the above part using RK4.

[1] In MATLAB, type 'help ode23s' and it will provide you information on how to use this solver. There are several other stiff solvers listed too. An example of stiff ode solver is posted on blackboard