Temple Math 5044 **Introduction to Numerical Analysis II** **Spring 2023**

Problem Set 5

(Out Thu 03/30/2023, Due Tue 04/18/2023)

Problem 8

As a baseline consider five chemicals with the following chemical reaction scheme

$$\mathrm{A} \underset{\lambda/2}{\overset{\lambda}{\rightleftharpoons}} \mathrm{B} \underset{\lambda/2}{\overset{\lambda}{\rightleftharpoons}} \mathrm{C} \underset{\lambda/2}{\overset{\lambda}{\rightleftharpoons}} \mathrm{D} \underset{\lambda/2}{\overset{\lambda}{\rightleftharpoons}} \mathrm{E}$$

where λ is the reaction rate parameter.

In addition, the concentration for each component (A,B,C,D,E) evolves according to the nonlinear reaction equation

$$u' = c(u) = \mu u(u-\beta)(1-u) \ ,$$

where μ determines the strength of the nonlinear reaction, and $0 < \beta < 1$ is a parameter.

We choose $\lambda = 10^4$, $\mu = 50$, and $\beta = 0.3$, final time $T = 1$, and initial concentrations of 1 for A and 0 for B, C, D, and E.

(a) Derive the 5-dimensional ODE system that describes the linear reactions (without the function c). Explain which dynamics are induced by those reactions.

(b) Plot the function $c(u)$, and based on its shape, explain how solutions to the ODE $u' = c(u)$ behave in time (classify equilibrium points), and the role of β.

(c) Write the full reaction dynamics in the form

$$u'(t) = f(t) = g(t) + h(t) \ ,$$

where g encodes the stiff linear λ-reactions, and h the nonlinear μ-reactions.

(d) Use RK4 with very small time steps (e.g., $k = 10^{-5}$) to produce the true solution of the full problem.

(e) Program at least 4 different ImEx methods that can solve the same problem with substantially larger time steps. Plot the resulting solutions (the five concentrations as functions of time) together with the RK4 reference solutions.

(f) Change the value of β to 0.4. You should observe a fundamental change of behavior of the solution. Using your best numerical method, determine, as accurately as possible, the critical value of β at which the behavior of the solution switches.

Problem 9

Download the Matlab program `temple5044_voyager.m` from the course web site, and modify it as follows: (i) remove the Voyager space probe, and instead add the planets Mercury, Venus, and Mars; (ii) insert the relevant parameters of these newly added planets, assuming a circular trajectory around the sun of a distance given by the semi-major axis; (iii) place the new planets initially on the line between the sun and Jupiter, with the initial velocities chosen as done for Jupiter; (iv) change the final time to be 100 Earth years, and the time step to be 5 Earth days.

Then implement three numerical methods: Heun's method, RK4, and the velocity Verlet method, and integrate the system up to the final time. For each numerical solution, plot the time-evolution of the following quantities: the distances between each planet and the sun; and the energy ratio $E(t)/E(0)$, where

$$E = \sum_{i=1}^{N} m_i |\vec{v}_i|^2 - \sum_{i \neq j} G m_i m_j |\vec{x}_i - \vec{x}_j|^{-1}$$

is the total energy of the N-body system (see the Matlab code and your resources for the values of the parameters).

Explain your observations, and discuss which properties of the numerical schemes are responsible for the structural observations.

Instructions

For each problem set, you need to submit one document, either in class or via email to the course instructor, that contains plots and explanations (hand-written or typed). If you decide to email the document, name it `yourfamilyname_problemset1.pdf`, where 1 stands for the number of the problem set.

In addition, for each programming task, email your respective program to the course instructor, under the filename `yourfamilyname_problem1a.m`, where `1` stands for the problem number and `a` for the sub-problem letter.