ESC113 Term Project

Group 7

24th June 2023

1 Kinetic Modelling and Optimisation of Series Reactions.

1.1 Problem Statement :

Determine the solution to the kinetic system :

- $A \longrightarrow B \longrightarrow C$
- $B \longrightarrow D$

where the reaction rates are k_1, k_2, and k_3 (in the order written here).The corresponding ODEs that you need to solve are :

- dA/dt $= -k_1 A$; dB/dt $= k_1 A - k_2 B - k_3 B$; dC/dt $= k_2 B$; dD/dt $= k_3 B$

Initial Conditions : $A(t = 0) = A_0$; $B(t = 0) = 0$; C(t=0) = 0; D(t=0) = 0;

1) Write a MATLAB program that plots the solution up to $t = 10$ for $k_1 = 2$, $k_2 = 0.5$, $k_3 = 0.3$, and $A_0 = 1$.

2) Now write a MATLAB program that use methods to solve the system.

3) Pick a time step so that the solution is stable and the error is small. Our program should plot the numerical solution and the analytical result together.

1.2 Implementation

1) Define discretisation.
2) Use centered finite difference at interior nodes to convert the ODE into a system of non-linear algebraic equations consistent with the boundary conditions.
3) Define residuals and the analytical Jacobian required for the Newton Raphson method.
4) Use the Newton-Raphson method to find roots.

Group 7 Members : Diya Saraf (220383), Ankit Kumar (220159), Suyash Jindal (221113) , Harshit Gupta (220439), Tushar Verma (221147), Divyanshu Chauhan (220380), Bhavishya Gupta (220295), Abhishek Kumar (220045), Saurabh Singh (220990).