DEPARTMENT OF MATHEMATICS IIT GUWAHATI

MA 332 Scientific Computing

Lab - VIII

1. Using the Runge-Kutta method of 2nd order, solve

$$y'(t) = -y(t) + t^{0.1}(1.1 + t), \quad y(0) = 0$$

whose solution is $y(t) = t^{1.1}$. Solve the problem on [0, 5], printing the solution and the errors at t = 1, 2, 3, 4, 5, use step sizes h = 0.005, 0.025, 0.0125, 0.00625, calculate the ratios by which the errors decrease when h is halved. How does this compare with the theoretical value of convergence of $O(h^2)$. explain your results as best you can.

2. Solve the initial-value problem

$$x' = x/t + t \sec(x/t), \quad x(0) = 0$$

by the fourth-order Runge-Kutta method. Continue the solution to t = 1 using step size $h = 2^{-7}$. Compare the numerical solution with the exact solution, which is $x(t) = t \arcsin t$. Define f(0,0) = 0, where $f(t,x) = x/t + t \sec(x/t)$.

3. The irreversible chemical reaction in which two molecules of solid potassium dichromate $(K_2Cr_2O_7)$, two molecules of water (H_2O) , and three atoms of solid sulfur (S) combine to yield three molecules of the gas sulfur dioxide (SO_2) , four molecules of solid potassium hydroxide (KOH), and two molecules of solid chromic oxide (Cr_2O_3) can be represented symbolically by the stoichiometric equation:

$$2K_2Cr_2O_7 + 2H_2O + 3S \rightarrow 4KOH + 2Cr_2O_3 + 3SO_2.$$

If n_1 molecules of $K_2Cr_2O_7$, n_2 molecules of H_2O , and n_3 molecules of S are originally available, the following differential equation describes the amount x(t) of KOH after time t:

$$\frac{dx}{dt} = k \left(n_1 - \frac{x}{2} \right)^2 \left(n_2 - \frac{x}{2} \right)^2 \left(n_3 - \frac{3x}{4} \right)^3$$

where k is the velocity constant of the reaction. If $k = 6.22 \times 10^{-19}$, $n_1 = n_2 = 2 \times 10^3$, and $n_3 = 3 \times 10^3$, use the Runge-Kutta method of order four to determine how many units of potassium hydroxide will have been formed after 0.2s?

- 4. Use Adams-Bashforth and Adams-Moulton methods to approximate the solutions to the following IVPs
 - (a) $y' = 1 + y/t + (y/t)^2$, $1 \le t \le 3$, y(1) = 0 with h = 0.002;
 - (b) $y'(t) = \sin(t) y$, $0 \le t \le 1$, y(0) = 1 with h = 0.005;

- i) Use exact starting values.
- ii) Use starting values obtained from the Runge-Kutta method of order four.

Compare the results to the actual values.

5. Using the Adams-Bashforth and Adams-Moulton methods, solve

$$y'(t) = -50y(t) + 51\cos(t) + 49\sin(t), \quad y(0) = 1$$

for $0 \le t \le 10$. The solution is $y(t) = \sin(t) + \cos(t)$. Use step sizes of h = 0.01, 0.001; In each case, print the errors as well as answers.