DEPARTMENT OF MATHEMATICS, I.I.T. GUWAHATI

MA 322: Scientific Computing Lab - VII

1. Use the methods mentioned below to approximate the solutions to each of the following initial-value problems, and compare the results to the actual values.

   (a) $y' = \dfrac{2-2ty}{t^2+1}$, $0 \le t \le 1$, $y(0) = 1$ with $h = 0.1$; actual solution $y(t) = \dfrac{2t+1}{t^2+1}$.

   (b) $y' = \dfrac{y^2+y}{t}$, $1 \le t \le 3$, $y(1) = -2$ with $h = 0.2$; actual solution $y(t) = \dfrac{2t}{1-2t}$.

   (c) $y' = 1 + y/t + (y/t)^2$, $1 \le t \le 3$, $y(1) = 0$ with $h = 0.2$; actual solution $y(t) = t\tan(\ln t)$.

   (d) $y' = e^(t - y)$, $0 \le t \le 1$, $y(0) = 1$ with $h = 0.5$; actual solution $y(t) = \ln(e^t + e - 1)$.

   1. Explicit-Euler method
   2. Implicit-Euler method
   3. Modified-Euler method
   4. Midpoint method
   5. Second and Fourth-order Runge-Kutta methods

2. Solve the initial-value problem $x' = x/t + t\sec(x/t)$ with $x(0) = 0$ 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:

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

   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 IVPs given in Question 1.

   (a) Use exact starting values.

   (b) Use starting values obtained from the Runge-Kutta method of order four.

   Compare the results to the actual values.