Lab 7: MA 322

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1. 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:

$$\frac{dy}{dx} = k\Big(n_1 - \frac{x}{2}\Big)^2\Big(n_2 - \frac{x}{2}\Big)^2\Big(n_3 - \frac{3x}{4}\Big)^3,$$

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 $0.2s$?

2. Show that the Runge-Kutta method of order second and the Modified Euler method give the same approximations to the initial-value problem

$$\frac{dy}{dt} = -y + t + 1, \;\; 0 \leq t \leq 1, \;\; y(0) = 1.$$

for any choice of h. Why is this true?

3. Use the Modified Euler method to approximate the solutions to each of the following initial-value problems, and compare the results to the actual values.

   (a) $\frac{dy}{dt} = \frac{1+t}{y+1}$, $\;1 \leq t \leq 2$, $\;y(0) = 1$, with $h = 0.5$; actual solution $y(t) = \sqrt{t^2 + 6 + 2t} - 1$.

   (b) $\frac{dy}{dt} = \frac{\sin 2t - 2ty}{t^2}$, $\;1 \leq t \leq 2$, $\;y(1) = 2$, with $h = 0.25$; actual solution $y(t) = \frac{4 + \cos 2 - \cos 2t}{2t^2}$.

4. Consider the problem

$$\frac{dy}{dt} = y - t^2 + 1, \;\; 0 \leq t \leq 2 \;\; y(0) = 0.5.$$

Use Euler's method with $h = 0.025$, the Runge-Kutta second-order method with $h = 0.05$, and the Runge-Kutta fourth-order method with $h = 0.1$ and compared at the common mesh points of these methods $0.1, 0.2, 0.3, 0.4$, and 0.5.

5. Consider the initial-value problem

$$\frac{dy}{dt} = y - t^2 + 1, \ \ 0 \le t \le 2, \ \ y(0) = 0.5.$$

Use the exact values given from $y(t) = (t+1)^2 - 0.5e^t$ as starting values and $h = 0.2$ to compare the approximations from

(a) by the explicit Adams-Bashforth four-step method.

(b) the implicit Adams-Moulton three-step method.

6. Use each of the Adams-Bashforth methods to approximate the solutions to the following initial-value problems. In each case use starting values obtained from the Runge-Kutta method of order four. Compare the results to the actual values.

(a) $\frac{dy}{dt} = \frac{2-2ty}{t^2+1}$, $\ 0 \le t \le 1$, $\ y(0) = 1$, with $h = 0.1$; actual solution $y(t) = \frac{2t+1}{t^2+1}$.

(b) $\frac{dy}{dt} = \frac{y^2}{t+1}$, $\ 1 \le t \le 2$, $\ y(1) - \ln(2)^{-1}$, with $h = 0.1$; actual solution $y(t) = \frac{-1}{\ln(t+1)}$.

(c) $\frac{dy}{dt} = \frac{y^2+y}{t}$, $\ 1 \le t \le 3$, $\ y(1) = -2$, with $h = 0.2$; actual solution $y(t) = \frac{2t}{1-t}$.

7. Apply the Adams fourth-order predictor-corrector method with $h = 0.2$ and starting values from the Runge-Kutta fourth order method to the initial-value problem

$$\frac{dy}{dt} = y - t^2 + 1, \ \ 0 \le t \le 2, \ \ y(0) = 0.5.$$

END