Problem Set for Module – 07

Dr. Niket S. Kaisare

Department of Chemical Engineering, Indian Institute of Technology Madras

Problem 1: Runge-Kutta RK-3 Method Derivation

The RK-3 method may be written as:

$$y^{i+1} = y^i + h(w_1 k_1 + w_2 k_2 + w_3 k_3) \quad \text{etc.}$$

Derive the conditions on the weights w_i, p_i and q_{ij} for the RK-3 method.

Problem 2: Comparison of RK-4 with Newton-Cotes Integration Formulae

Show that the solution to $y' = f(y,t)$ using the standard RK-4 method reduces to a Simpson's rule if the right hand side is only a function of t, i.e., for $y' = f(t)$.

Problem 3: Region of Stability

Find the region of stability for RK-2 method for solution to the problem $y' = -\lambda y$.

Problem 4: Implicit and Explicit Euler's Methods

Solve the ODE below using Implicit and Explicit Euler's methods with $h = 1$ in the range $t = [0,2]$:

$$\frac{dy}{dt} = -5ty \qquad y(0) = 1$$

Problem 5: Explicit Euler's Method

Reduce the step size h until you achieve a stable solution using Euler's explicit method.

Problem 6: Runge-Kutta Methods

For the step size used in the previous problem, solve the ODE-IVP using RK-2, RK-3 and RK-4 methods. Compare with the true solution.

Problem 7: Effect of Step Size

1. For either of the Euler's methods (implicit or explicit), reduce the step size until the solution $y(t)$ in the entire domain (i.e., the error in numerical and true values for $t \in [0,2]$) is accurate to $E_{tol} = 10^{-3}$.
2. Repeat for the RK-2 method of your choice
3. Repeat for the standard RK-4 method
4. Compare the minimum step size required for the desired accuracy with the three methods. Also comment on the accuracy of the solution using the ODE solving techniques.

Problem 8: Predictor-Corrector Method

Solve the example above using Heun's Predictor-Corrector method for a step size of $h = 0.1$. Use three iterations of the Corrector Equation.

Problem 9: Crank-Nicholson Method

Solve the example above using Crank-Nicholson Method.

Problem 10: Adam's Method

Solve the example above using Adam's method. Use Heun's method solution (from Problem 8: above) to start Adam's method.

Problem 11: More examples

Repeat Problems 7 to 10 for the following examples:

1. $y' = y\sin(t)$ for $t \in [0,1]$ with $y(0) = 1$

APPLICATIONS

Problem 12: Multi-Variable Problem: The Lorenz Equation

Consider the Lorenz Attractor, described by the following equations:

$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = rx - y - xz \text{ , where } \sigma = 10 \text{ and } b = 8/3$$
$$\dot{z} = xy - bz$$

Lorenz used the value $r = 28$ to demonstrate chaos. We will use the following procedure:

1. Choose an arbitrary point `y0` in the state space, which will be the initial condition
2. Run simulations until t = 25
3. Plot the results of *x*, *y* and *z* as a function of time *t*.
4. Repeat for another initial condition which is slightly different from y0 chosen above. (e.g., use $y_{0,\text{new}} = 1.001 \times y_{0,\text{old}}$)

Problem 13: Curing of Thermo-Setting Polymer

Initial polymer is often "sticky" so that it can be appropriately moulded into desired shapes. Once put in a mould, the polymer is thermally treated. This *curing* process "sets" the polymer in the appropriate shape and gives it appropriate physical properties (strength, thermal resistance, etc.). In general, the curing process is very complex and involves several reactions and heat effects. However, we will simplify these reactions for this problem. We will use the mechanism of Ding and Leonov (Rubber Chemistry and Technology, 1996) for this purpose. The reactions include:

$$A \overset{k_1}{\rightarrow} B \overset{k_2}{\rightarrow} B^* \overset{k_3}{\rightarrow} P \overset{k_4}{\rightarrow} D$$

$$B^* \overset{k_5}{\rightarrow} D$$

In the above reactions, P is the desired product and D are undesired side-products (called "Dead-Ends"). The rate constants (in min^{-1}) are given by:

	$A \xrightarrow{k_1} B$	$B \xrightarrow{k_2} B^*$	$B^* \xrightarrow{k_3} P$	$P \xrightarrow{k_4} D$	$B^* \xrightarrow{k_5} D$
Pre-Exponential	1.44×10^9	2.727×10^{13}	5.131×10^{17}	4.95×10^{25}	6.48×10^{19}
E_{act}/R	9.73	13.32	16.16	27. 86	17.60

Consider an isothermal batch operation at 140 °C. Obtain concentrations of all species A, B, B^*, P, D with time. The initial concentration of A is 250 mol/m^3. Run the simulations from 0 to 80 minutes.

Problem 14: Transients in a CSTR (multiple variables)

Consider a CSTR wherein the following reactions take place:

$$A \rightarrow 2B \qquad -r_1 = k_1 c_A$$

$$A \rightleftharpoons C \qquad -r_2 = k_2 c_A^{1.5}; -r_{-2} = k_{-2} c_C^2$$

$$B \rightarrow C + D \qquad -r_3 = k_3 c_B^2$$

Given: $k_1 = 1$; $k_2 = 0.2$; $k_{-2} = 0.05$; $k_3 = 0.4$; $C_{A0} = 1$; V/F = 2. Starting initially with $C_A(t = 0) = 1.0$, obtain how concentrations of A, B, C, D vary with time.

Problem 15: Dhoni's Sixes and the Dharmasala Effect

After hitting Irfan Pathan for consecutive sixes that ensured Chennai's entry into the semis of IPL-3, the captain M. S. Dhoni remarked that it was easier to hit sixes in Dharmasala (1.2 km above sea level) than it would be in Mohali (assume sea level for this problem). The overall model for the system, obtained from Newton's laws of motion, is given by

$$x'' = -cvx' \quad \text{and} \quad y'' = -cvy' - g$$

In the above equations, x and y are horizontal and vertical locations; $v = (x')^2 + (y')^2$ is the velocity magnitude; c is the drag constant and g is the gravitational acceleration.

The earth's gravitational acceleration at Mohali is 9.81 m^2/s and the drag coefficient is $c = 0.006$.

- If Dhoni hit the ball at 35 m/s with a 45° angle, find the distance ball travels in Mohali.
- What will be the distance travelled by the ball in Dharmasala?

The gravitational acceleration varies with height as

$$\frac{g_h}{g_{\text{Mohali}}} = \left(\frac{R_e}{R_e + h}\right)^2 \quad \text{where} \quad R_e = 6400$$

whereas, the drag constant varies with height as:

$$\frac{c_h}{c_{Mohali}} = \left(1 - \frac{6.5h}{300}\right)^5$$