CHL711 - Numerical Methods in Chemical Engineering

Time : 2½ hours
Max. Marks : 90

Date: 28. 11. 2006

Major Examination

Part A (32 Marks)

1. Briefly state what is involved in cubic spline interpolation. 3

2. Obtain the value of the integral $\int_2^3 (x \ln x)\,dx$ after reducing it to the form $\int_{-1}^{1} f(z)\,dz$ and using the 3-point ($n=2$) Gauss–Legendre quadrature, i.e. $P_3(x) = \frac{1}{2}(5x^2 - 3x)$. The weights w_i are 0.889 for the middle z_i and 0.556 for the other two. 5

3. Why do Adams-Bashforth formulae for ODE-IVP use backward differences $\nabla^j y$? 2

4. Derive the second order Runge-Kutta algorithm for ODE-IVP (modified Euler, etc); are these explicit or implicit ? 7

5. For ODE-IVP, can the numerical solutions be more than one? How is the correct one decided? What is the condition for numerical stability? 4

6. What is stiffness ratio ? What does it imply for step-size ? 3

7. In OC technique, for symmetric solution of the ODE why is the $x=0$ condition not utilized ? 3

8. What do you understand by orthogonal collocation on Finite Elements (OCFE)? Why is it required 3

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Part B (58 Marks)

1. Consider the following coupled equations [12]

$$x^2 + y^2 - 4 = 0 \quad \text{and} \quad x^2 - y^2 - 1.5 = 0$$

(Do not eliminate variables to give $x^2 = 2.75$ and $y^2 = 1.25$). Obtain the algorithm to solve for x and y using the two-variable Newton Raphson method. Obtain the inverse of the Jacobian analytically. Starting with x =1 and y = 1, obtain two iterates and compare with the analytical solution.

2. Consider the Legendre polynomial $P_3(x) = ½ (5x^3 - 3x)$. Generate a set of four data points corresponding to base points x = -1.0, -0.4, 0.5, 1.0 . Fit a 2nd degree (using first three data points) as well as a 3rd degree polynomial using Lagrangian interpolation. Compare the fitted polynomials and the exact results at x = 1.0 . [10]

3. (i) Using the approximation to $y'(\alpha)$ in terms of the backward differences $\nabla^j y$, derive the 2nd and 4th order (j=1 and j=3) Adams-Bashforth formulae for integrating ODE-IVP.

   (ii) For the differential equation given below

$$dy/dt = y - t^2 \; ; \; y(0) = 1 \; ; \; y(0.2) = 1.2186 \; ; \; y(0.4) = 1.4682 \; ; \; y(0.6) = 1.7379$$

   using both formulae obtain y(1.0). Estimate the errors. Compare with analytical solution if possible. [10]

4. Consider the 2nd order Gear *corrector* equation. Obtain its characteristic roots and study its stability in terms

   (a) spurious roots. Find out which one is the correct root.
   (b) Propagation of the round off errors. [8]

$$(1 + x)^{½} = 1 + x^2/2 - x^2/8 + \ldots.. \; ; \; (1 + x)^{-1} = 1 + x + x^2 + x^3 + \ldots\ldots \; ; \; e^x = 1 + x + x^2/2 + x^3/3! + \ldots.$$

5. (a) Solve the following differential equation, using the N =2 orthogonal collocation procedure along with NR method. Get $y^{(2)}$ and $y^{(3)}$.

$$d^2y/dx^2 + dy/dx - y = e^y \quad ; \quad y(0) = 0 \text{ and } y(1) = 0 \; ; \; \text{NR start } y^{(1)} = [0.1, 0.2]^T$$

   (b) Consider the ODE-BVP

$$d^2y/dx^2 - 2y^3 = 0 \; ; \; y(0) = 1 \text{ and } [\, dy/dx + y^2 \,]_{x=1} = 0$$

   Set up the final NR equations to be solved for N=1 OC technique. [18]