1/5/15

(1) (26)

Comp Programming & numerical mthds
CHEM/CBGS/III/CNM

(REVISED COURSE)
(3 Hours)

QP Code :4908

[Total Marks: 80

N.B. :

1) Question – 1 is compulsory. Answer any three questions from remaining.
2) Assume data if necessary and specify the assumptions clearly
3) Draw neat sketches wherever required.
4) Answer to the sub-questions of an individual question should be grouped and written together i.e. one below the other.

1. (a) Consider the following system of equations: [10]

$$\begin{bmatrix} 1 & 1 \\ 1 & (1+\epsilon) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \end{bmatrix}$$

Solve the system for $\epsilon = 0.01$; 0.001; and 0.0001 by elimination. How sensitive is the solution to changes in ϵ?

(b) Use Crank-Nicholson Scheme to solve, [05]

$$u_{xx} = u_t \qquad 0 \le x \le 1 \qquad t > 0 \qquad h = \frac{1}{4} \qquad k = \frac{1}{4}$$

Given $u(x,0) = 0$, $u(0,t) = 0$, $u(1,t) = 50t$ Compute u for one step in t-direction.

(c) Explain how to use 'for' loop in SciLab with appropriate example. [05]

2. (a) Consider the following equation: [12]

$$f(x) = x^3 - 5x^2 + 6x - 1 = 0$$

Rewriting this as:

$$x = x + f(x) = g(x)$$

Start from $x^{(0)} = 0$ and compute upto $x^{(3)}$, by Successive Substitution. What happens if we start with $x^{(0)} = 1$. Is convergence guaranteed, for $0 \le x \le 3$?

(b) Solve the following system by LU decomposition: [08]

$$\begin{bmatrix} 1 & -1 & 2 \\ 2 & -2 & 3 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -8 \\ -20 \\ -2 \end{bmatrix}$$

3. (a) Obtain a root of the following equation using Newtons Method in the interval $0 \le x \le 2$: [12]

$$f(x) = \ln(x^2 + 1) - e^{0.4x}\cos(\pi x)$$

(b) Solve the following equation to find a root in the interval [0.1, 2] by the method false position. Obtain a value correct to three decimal places. [08]

4. (a) Find $x(2)$ from following ODE using fourth order Runge-Kutta method: [14]

$$\frac{dx}{dt} = e^{-t}(\cos t - \sin t) - \sin(\frac{t}{2}) \qquad \text{with} \qquad x(0) = 2$$

(b) Write Laplace equation and express it in difference form using Taylor's series expansion [06]

5. Solve the following equations using Newtons Method and starting from [20]

$$x^{(0)} = \begin{bmatrix} 0.1 \\ 0.2 \end{bmatrix}$$

$$f_1(x) = x_1^2 x_2 + x_2^2 x_1 - 2x_1 x_2 + 5x_1 - 7 = 0$$
$$f_2(x) = x_1^3 - 2x_1^2 x_2^2 + x_1 x_2^2 - 6x_2 + 15 = 0$$

Perform minimum three iterations.

6. (a) Consider the following example: [12]

$$\frac{dy}{dt} = -y^2 \qquad \text{with} \qquad y = 1 \qquad \text{at} \qquad t = 0$$

where t and y are scaled variables. This equation represents a second order reaction taking place in a tubular reactor. Integrate the equation using Eulers Implicit Method from $t = 0$ to $t = 5$.

(b) Solve the following system by Jacobi Iteration: [08]

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Carry out five iterations.

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