GIET UNIVERSITY, GUNUPUR – 765022

Numerical Method in Chemical Engineering

B.Tech (IV Sem. – Regular) Examinations, April/May – 2021

NM – (Set-1) / Answer Scheme

PART – A

Q.1)

(a) (i) – Smaller interval

(b) (iii) – 2

(c) (i) – Iterative method

(d) (iii) – Dominant

(e) (iii) – It does not guarantee the convergence of each and every matrix

(f) (i) – Differential equations

(g) (iii) – 1

(h) (ii) – $\frac{14h}{45} \Delta^4 y_0$

(i) (ii) – False

(j) (iv) – 4

PART - B

(2x10 = 20)

(a) let $x = \sqrt{12} \Rightarrow f(x) = x^2 - 12$

$f(3) = -ve; \; f(4) = +ve$

Take $x_0 = 3$, $\quad x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = 3 - \frac{f(3)}{f'(3)} = 3.5$

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} = 3.5 - \frac{(3.5)^2 - 12}{2(3.5)} = 3.4642$$

Hence, the root is 3.4642

(b)

Order of convergence is two.

The convergence condition is,

$$|f(x) \cdot f''(x)| < |f'(x)^2|$$

(c) When the function is given in the form of values with table instead of given analytical expression, we use numerical differentiation.

(d)

$$f'(x) = \frac{1}{h}\left[\Delta y_0 + \frac{2r-1}{2}\Delta^2 y_0 + \frac{3r^2-6r+2}{6}\Delta^3 y_0 + \cdots\right]$$

(f) The Crank - Nicholson formula is

$$u_{i+j} - 4u_{i,j+1} + u_{i-1,j+1} = u_{i+1,j} - u_{i-1,j}$$

(e)

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

(ie) $u_t = u_{xx}$

(ie) $u_{xx} - u_t = 0$

The explicit formula to solve this equation is,

$$u_{i,j+1} = \frac{1}{2}\left[u_{i+1,j} + u_{i-1,j}\right]$$

(g)

$$\frac{\partial^2 u}{\partial t^2} = \frac{u_{i,j-1} - 2u_{i,j} + u_{i+1,j}}{k^2}$$

(h) Given $x_0 = 0, y_0 = 1$; $\frac{dy}{dx} = x^2 + y^2$

Modified Euler's formula is,

$$y_{n+1} = y_n + h\, f\left[x_n + \frac{h}{2}, y_n + \frac{h}{2} f(x_n, y_n)\right]$$

Now, $f(x_0, y_0) = x_0^2 + y_0^2 = 1$

$$y_0 + \frac{h}{2} f(x_0, y_0) = 1 + \frac{0.1}{2}(1) = 1.05$$

$$f\left[x_0 + \frac{h}{2}, y_0 + \frac{h}{2} f(x_0, y_0)\right] = f(0.05, 1.05)$$

Then,

$$f(0.05, 1.05) = (0.05)^2 + (1.05)^2 = 1.1105$$

Hence, $y(0.1) = 1.1105$

(i) The fourth order Runge-Kutta method agree with Taylor series solution upto the terms of h^4. Hence, it is called fourth order R-K method.

(j) (i) To use Adam's method, we need at least four values of 'y' prior to the required value of 'y'.

(ii) In the corrector formula, the value of y'_{n+1} is obtained by using the predictor value of y_{n+1}.

(k)

$$k_1 = h f(x_0, y_0)$$

$$k_2 = h f\left(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}\right)$$

$$\therefore \Delta y = k_2.$$

That is, $y_1 = y_0 + \Delta y$

PART-C

3-(a) From the given system of eqns, we can write,

$$x = -3+2y \quad ; \quad y = \frac{1}{25}[15 - 2x]$$
— (3) — (4)

1st iteration

Put $y=0 \xrightarrow{(3)} x=-3$

Put $x=-3 \xrightarrow{(4)} y = \frac{1}{25}[15-2(-3)] = 0.84$

Hence, $x=-3$, $y=0.84$

llly,

2nd iteration

$x = -1.32$, $y = 0.7056$

3rd iteration

$x = -1.589$, $y = 0.727$

4th iteration

$x = -1.5246$, $y = 0.724$

5th iteration

$x = -1.552$, $y = 0.724$

6th iteration

$x = -1.552$, $y = 0.724$

Hence, the soln. is,

$x = -1.552$

$y = 0.724$

(3) -(b)

N-R formula is,

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \quad \text{—(1)}$$

For $n=0$, (1) $\Rightarrow x_1 = 0.25$

For $n=1$, (1) $\Rightarrow x_2 = 0.2586$

For $n=2$, (1) $\Rightarrow x_3 = 0.2586$

Hence, the smallest positive root is $\underline{x = 0.2586}$

(3) -(c) The given system of equations can be written as

$$x = \tfrac{1}{4}(14 - 2y - z) \quad \text{—(4)}$$

$$y = \tfrac{1}{5}(10 - x + z) \quad \text{—(5)}$$

$$z = \tfrac{1}{8}(20 - x - y) \quad \text{—(6)}$$

<u>1st iteration</u>

$x = 3.5$, $y = 1.3$, $z = 1.9$

<u>2nd iteration</u>

$x = 2.375$, $y = 1.905$, $z = 1.965$

<u>3rd iteration</u>

$x = 2.056$, $y = 1.982$, $z = 1.995$

4th iteration

$x = 2.010, \quad y = 1.997, \quad z = 1.999$

5th iteration

$x = 2.001, \quad y = 1.999, \quad z = 2$

6th iteration

$x = 2.001, \quad y = 1.999, \quad z = 2.$

Hence, the reqd. soln. is

$x = 2.001$

$y = 1.999$

$z = 2$

(3) - (d) $f(0) = +ve \; ; \; f(1) = -ve$

$\Rightarrow$ The roots lies between 0 and 1

N-R formula is

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Also, $|f(1)| < |f(0)| \Rightarrow$ The required root is nearer to 1.

For $n=0$, $x_1 = 0.67$

For $n=1$, $x_2 = 0.73$

For $n=2$, $x_3 = 0.73$

So, the required root is $\underline{x = 0.73}$

4 -(a) The given system can be written as

$$x = \frac{1}{41}(65.46 + 2y - 3z)$$

$$y = -\frac{1}{27}(71.31 - x - 2z)$$

$$z = \frac{1}{52}(173.61 - x - 3y)$$

Given $x=1,\ y=-2,\ z=3$.

1st iteration $x = 1.2795,\ y = -2.3715,\ z = 3.4509$

2nd iteration

$x = 1.2284,\ y = -2.3399,\ z = 3.450$

3rd iteration

$x = 1.23,\ y = -2.34,\ z = 3.45$

4th iteration

$x = 1.23,\ y = -2.34,\ z = 3.45$

The reqd. solns. are

$x = 1.23$
$y = -2.34$
$z = 3.45$

(4) -(b) $f(x) = \cos x - xe^x$; $f'(x) = -\sin x - [xe^x + e^x]$

and $x_0 = 0.5$

The N-R formula is

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \quad \text{--- (1)}$$

For $n=0$, $x_1 = 0.5181$

For $n=1$, $x_2 = 0.5178$

For $n=2$, $x_3 = 0.5178$

Hence, the required root is $\underline{0.5178}$.

(4)-(c) The given system can be written as

$$x = \frac{1}{8}(18+y-z)$$

$$y = \frac{1}{5}(3-2x+2z)$$

$$z = \frac{1}{3}(6+x+y)$$

1st iteration $x = 2.25$, $y = -0.3$, $z = 2.65$

2nd iteration $x = 1.8813$, $y = 0.9075$, $z = 2.9296$

3rd iteration $x = 1.9972$, $y = 0.9729$, $z = 2.9900$

4th iteration $x = 1.9979$, $y = 0.9968$, $z = 2.9982$

5th iteration $x = 1.9998$, $y = 0.9994$, $z = 2.9997$

6th iteration $x = 1.9999$, $y = 0.9999$, $z = 2.9999$

Hence, the required solns. are: $x=1.9999$, $y=0.9999$, $z=2.9999$

(4) - (d) Let $x = \sqrt{K} \Rightarrow f(x) = x^2 - K = 0$

$$f'(x) = 2x$$

The N-R formula is

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \quad \text{--- (1)}$$

$$\Rightarrow x_{n+1} = x_n - \left[\frac{x_n^2 - K}{2x_n}\right]$$

$$= x_n - \frac{x_n}{2} + \frac{K}{2x_n} = \frac{x_n}{2} + \frac{K}{2x_n}$$

(ii) $$x_{n+1} = \frac{1}{2}\left[x_n + \frac{K}{x_n}\right] \quad \text{--- (2)}$$

To find the value of $\sqrt{5}$

The root lies between 2 and 3

For $n=0$, $x_1 = 2.25$

For $n=1$, $x_2 = 2.2361$

For $n=2$, $x_3 = 2.2361$

Hence the required root is 2.2361

~~(5)~~ (5) – (a)

The modified Euler's algorithm is

$$y_{n+1} = y_n + h f\left[x_n + \frac{h}{2},\ y_n + \frac{h}{2} f(x_n, y_n)\right] \quad \text{—(1)}$$

Put $n=0$ in (1) $\Rightarrow$ $f(x_0, y_0) = \log(x_0 + y_0) = \log 2$
$= 0.3010$ —(2)

(2) in (1) $\Rightarrow$ $y_1 = 2 + 0.2 f\left[0.1,\ 2 + 0.1(0.3010)\right]$

Now, $f(0.1, 2.0301) = \log(0.1 + 2.0301) = 0.3284$ —(3)

(3) in (2) $\Rightarrow$ $y_1 = 2 + 0.2(0.3284)$

$= 2.0657$

Hence, $y(0.2) = 2.0657$

(5) – (b) Adam's – Bashforth predictor formula is

$$y_{n+1,p} = y_n + \frac{h}{24}\left[55 y_n' - 59 y_{n-1}' + 37 y_{n-2}' - 9 y_{n-3}'\right] \quad \text{—(1)}$$

Given $x_0 = 1,\ y_0 = 1$ and $h = 0.1$

$x_1 = 1.1,\ y_1 = 1.233$

$x_2 = 1.2,\ y_2 = 1.548$

$x_3 = 1.3,\ y_3 = 1.979$

$x_4 = 1.4,\ y_4 = ?$

$$y_{4,p} = y_3 + \frac{h}{24}\left[55 y_3' - 59 y_2' + 37 y_1' - 9 y_0'\right]$$

Now, $y_0' = 2,$

$y_1' = 2.70193$

$y_2' = 3.66712$

$y_3' = 5.03457$

$\Rightarrow \boxed{y_{4,p} = 2.58372}$

Adam's - Bashforth Corrector formula is

$$y_{n+1,c} = y_n + \frac{h}{24}\left[9y'_{n+1} + 19y'_n - 5y'_{n-1} + y'_{n-2}\right]$$

$$\Rightarrow y_{4,c} = y_3 + \frac{h}{24}\left[9y'_4 + 19y'_3 - 5y'_2 + y'_1\right]$$

$$\Rightarrow \boxed{y_{4,c} = 2.57641}$$

(5) - (c)

The modified Euler's algorithm is,

$$y_{n+1} = y_n + h\, f\left[x_n + \frac{h}{2}, y_n + \frac{h}{2} f(x_n, y_n)\right]$$

For $n=0$, $y_1 = y_0 + h\, f\left[x_0 + \frac{h}{2}, y_0 + \frac{h}{2} f(x_0, y_0)\right]$

$$\Rightarrow y_1 = 1 + (0.1)\, f(0.05, 1.05)$$

$$\Rightarrow y(0.1) = 1.1105$$

Consequently, for $n=2$, $y_2 = 1.25026$

Hence $y(0.2) = 1.25026$

The required soln. is

x	0	0.1	0.2
y	1	1.1105	1.25026

(5) -(d) Given, $x_0 = 1.3$ $y_0 = 1.36412$

$x_1 = 1.2$ $y_1 = 1.22787$

$x_2 = 1.1$ $y_2 = 1.10681$

$x_3 = 1.0$ $y_3 = 1$, $y_4 = ?$ and $h = -0.1$

$x_4 = 0.9$

Adam's - Bashforth Predictor formula is

$$y_{n+1,p} = y_n + \frac{h}{24}\left[55y_n' - 59y_{n-1}' + 37y_{n-2}' - 9y_{n-3}'\right]$$

$$\Rightarrow y_{4,p} = y_3 + \frac{h}{24}\left[55y_3' - 59y_2' + 37y_1' - 9y_0'\right] \quad \text{—(1)}$$

$\Rightarrow$ $y_0' = 1.44176$,

$y_1' = 1.284987$

$y_2' = 1.137847$

$y_3' = 1$

$\Rightarrow$ $\underline{y_{4,p} = 0.906518}$

Adam's - Bashforth Corrector formula,

$$y_{n+1,c} = y_n + \frac{h}{24}\left[9y_{n+1}' + 19y_n' - 5y_{n-1}' + y_{n-2}'\right]$$

$\Rightarrow$ $\underline{y_{4,c} = 0.906520}$

(6) -(a) (i) When $h = 0.5$, $y = \frac{1}{1+x}$ $\Rightarrow$

x	0	0.5	1
y	1	0.6666	0.5

$\Rightarrow I_1 = 0.7083$

(ii) When $h = 0.25$, $y = \frac{1}{1+x}$ $\Rightarrow$

x	0	0.25	0.5	0.75	1
y	1	0.8	0.6666	0.5714	0.5

$\Rightarrow I_2 = 0.697$

(iii) When $h = 0.125$, $y = \frac{1}{1+x}$ $\Rightarrow$

x	0.125	0.25	0.375	0.5	0.625	0.75	0.875	1
y	0.8889	0.8	0.7272	0.6667	0.6153	0.5714	0.5333	0.5

$\Rightarrow I_3 = 0.6941$

Using Romberg's formula, $I = I_2 + \left(\frac{I_2 - I_1}{3}\right)$

$\Rightarrow I = 0.6931$

Now $\int_0^1 \frac{1}{1+x}\,dx = 0.693 \Rightarrow \left[\log(1+x)\right]_0^1 = 0.693$

$\Rightarrow \log_e 2 - \log 1 = 0.693$

(ie) $\log_e 2 = 0.693$

(6) – (b) R–K method

Given $y' = x + y$,

Now, $K_1 = h f[x_0, y_0] = h[x_0 + y_0] = 0.1$

$\Rightarrow K_2 = 0.11 \quad \left(K_2 = h f\left[x_0 + \frac{h}{2}, y_0 + \frac{K_1}{2}\right) \right.$

$\Rightarrow K_3 = h f(x_0 + h, y_0 + 2K_2 - K_1) = 0.122$

$\Rightarrow \Delta y = \frac{1}{6}[K_1 + 4K_2 + K_3] = \frac{1}{6}(0.662) = 0.1103$

$\Rightarrow y_1 = 1.1103$

To find $y(0.2)$: $x_0 = 0.1$, $y_0 = 1.1103$, $h = 0.1$

$K_1 = 0.12103$

$\Rightarrow K_2 = 0.13208$

$\Rightarrow K_3 = 0.14534$

$\Rightarrow \Delta y = 0.1324$

Hence $y_2 = y_1 + \Delta y = 1.2427$

(ie) $y(0.2) = 1.2427$

(6) -(c)

Let $y = \frac{1}{x^2+4}$

(i) when $h=1$, $y = \frac{1}{x^2+4} \Rightarrow$

x	0	1	2
y	0.25	0.20	0.125

By Trapezoidal rule

$$I_1 = \frac{h}{2}\left[(y_0+y_2)+2(y_1)\right] = 0.3875$$

(ii) When $h=0.5$, $y = \frac{1}{x^2+4} \Rightarrow$

x	0	0.5	1	1.5	2
y	0.25	0.2353	0.20	0.160	0.125

By Trapezoidal rule,

$$I_2 = \frac{h}{2}\left[(y_0+y_4)+2(y_1+y_2+y_3)\right] = 0.3914$$

(iii) When $h=0.25$, $y = \frac{1}{x^2+4} \Rightarrow$

x	0	0.25	0.5	0.75	1	1.25	1.50	1.75	2.00
y	0.25	0.2462	0.2353	0.2192	0.20	0.1798	0.160	0.1416	0.125

By Trapezoidal rule,

$$I_3 = \int_0^2 \frac{dx}{x^2+4} = \frac{h}{2}\left[(y_0+y_8)+2(y_1+y_2+y_3+y_4+y_5+y_6+y_7)\right]$$

$\Rightarrow I_3 = 0.3924$

Using Romberg's formula, for I_1 and I_2

$$I = I_2 + \left(\frac{I_2 - I_1}{3}\right) = 0.3927 \quad \text{—(1)}$$

For I_2 and I_3

$$I = I_3 + \left(\frac{I_3 - I_2}{3}\right) = 0.3927 \quad \text{—(2)}$$

from (1) and (2),

$$I = \int_0^2 \frac{dx}{4+x^2} = \frac{1}{2}\left[\tan^{-1}\left(\frac{x}{2}\right)\right]_0^2$$

$$= \frac{\pi}{8}$$

$$\Rightarrow \boxed{\pi \simeq 0.31416}$$

Note: for this problem, the weightage of full marks can be given to Romberg's method

(6)-(d)

Given $y' = y^2 + xy$.

By R-K method,

$$k_1 = h[f(x_0, y_0)] = 0.2$$

$$k_2 = hf\left[x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}\right] = 0.2365$$

$$K_3 = hf(x_0+h, y_0+2K_2-K_1) = 0.30208$$

$$\Delta y = \frac{1}{6}(K_1+4K_2+K_3) = 0.24135$$

$$y_1 = y_0 + \Delta y$$

(ie) $y(1.1) = 1.24135$

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(7)-(a)

The given eqn. can be written as:

$$u_{xx} = 16\, u_t$$

Here, $h = 1/4$, $a = 16$

choose $k = 1 \Rightarrow \lambda = \frac{k}{h^2 a} = 1$

The Crank-Nicolson formula is

$$\lambda u_{i+1,j+1} - (2\lambda+2)u_{i,j+1} + \lambda(u_{i-1,j+1})$$

$$= -\lambda u_{i+1,j} + (2\lambda-2)u_{i,j} - \lambda u_{i-1,j}$$

Substituting $\lambda = 1$, we get,

$$u_{i+1,j+1} - 4u_{i,j+1} + u_{i-1,j+1} = -u_{i+1,j} - u_{i-1,j}$$

Put $i=1, j=0$ $\quad u_{21} - 4u_{11} + 0 = 0 - 0 = 0$

Put $i=2$ and $j=0$

$$u_{31} - 4u_{21} + u_{11} = 0 - 0 = 0$$

Put $i=3, j=0$ we get,

$$u_{31} - 4u_{21} + u_{11} = 0$$
$$100 - 4u_{31} + u_{21} = 0$$

$\Rightarrow \quad u_{21} = 4u_{11} \quad (\text{or}) \quad u_{11} = \frac{1}{4} u_{21}.$

Then,

$$u_{31} - 4u_{21} + \frac{1}{4} u_{21} = 0$$

$$\Rightarrow u_{21} = \frac{-100}{-14} = 7.1428$$

Then,

$$-4u_{31} + 7.1428 = -100$$

$$\Rightarrow u_{31} = \frac{-107.1428}{-4} = 26.78$$

Hence,

$$u_{11} = 1.7857$$
$$u_{21} = 7.1428$$
$$u_{31} = 26.78$$

(7)-(b)

The given equation can be written as

$$y''(x) - y(x) = x \longrightarrow (1)$$

Using central difference approximation, we have,

$$y'' = \frac{y_{k-1} - 2y_k + y_{k+1}}{h^2}$$

Putting $k=1,2,3$ in (1), we get,

$$16y_0 - 33y_1 + 16y_2 = \frac{1}{4}$$

$$16y_1 - 33y_2 + 16y_3 = \frac{1}{2}$$

$$16y_2 - 33y_3 + 16y_4 = \frac{3}{4}$$

Since $h = 1/4$, we get

$$\Rightarrow x_1 = \frac{1}{4},\ x_2 = \frac{1}{2},\ x_3 = \frac{3}{4}$$

Solving from the above system, we have,

$$y_1 = -0.03488$$

$$y_2 = -0.05632$$

$$y_3 = -0.05004$$

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(7) - (c)

Here, $h=1$, $a=1$ and $k=1$

$$\Rightarrow \lambda = \frac{k}{h^2 a} = 1$$

The Crank - Nicolson formula when $\lambda = 1$, we have

$$u_{i-1,j} + u_{i+1,j} = 4u_{i,j+1} - u_{i+1,j+1} - u_{i-1,j+1} \quad \text{(1)}$$

Using condition $u(x,0) = \frac{x}{3}(16 - x^2)$, we get

$$u_{i,0} = \frac{i}{3}(16 - i^2)$$

$u_{1,0} = 5, \; u_{2,0} = 8, \; u_{3,0} = 7$

The values along x-axis at

$u_{10} = 5, \; u_{20} = 8, \; u_{30} = 7,$

Putting $i = 1, \; j = 1$ in (1), we get

$$-0 + 4u_{11} - u_{21} = 0 + 8$$

Solving the equations,

$$4u_{11} - u_{21} = 8$$

$$u_{11} - 4u_{21} + u_{31} = -12$$

$$u_{21} - 4u_{31} = -8$$

$$4u_{11} - u_{21} = 8$$

$$u_{21} - 4u_{31} = -8$$

$$4u_{11} - 4u_{31} = 0$$

$$u_{11} = u_{31}$$

Proceeding in the same way, we can get,

$$u_{12} = 1.7551$$

$$u_{22} = 2.4490$$

$$u_{32} = 1.7551$$

(7)—(d)

The given differential eqn. can be written as

$$y''(x) + y(x) + 1 = 0$$

Using the central difference approximation, we have,

$$y''(x) = \frac{y_{k-1} - 2y_k + y_{k+1}}{h^2}$$

Putting $k = 1, 2, 3,$ (i.e $h = 1/4$, $h = 1/2$ and $h = 3/4$), we get,

$$16y_0 - 31y_1 + 16y_2 + 1 = 0$$

$$16y_1 - 31y_2 + 16y_3 + 1 = 0$$

$$16y_2 - 31y_3 + 16y_4 + 1 = 0.$$

Applying the boundary conditions $y(0) = y(1) = 0$ and iterating the above system of equations,

we have, $y_1 = 0.10467$

$$y_2 = 0.1403$$

$$y_3 = 0.10467$$

And $y(0.5) = 0.1403$

— End of the Scheme —