BITS PILANI, DUBAI CAMPUS
DUBAI INTERNATIONAL ACADEMIC CITY, DUBAI

SECOND SEMESTER 2012-13
CHE F242 NUMERICAL METHODS FOR CHEMICAL ENGINEERS
COMPREHENSIVE EXAMINATION

Weightage: 40%
Max. Marks: 40

Date: 05.06.2013
Time: 12.30 PM – 3.30 PM

Answer all the questions.
No programmable calculators are allowed.

1. Using the Taylor's series 2nd order approximation to find f at $x = \frac{\pi}{3}$ with the base point at $x = \frac{\pi}{4}$ and calculate the relative percentage error: given $f(x) = \cos x$. (3M)

2. Solve $xe^x = \cos x$ by the method of false position, correct to 3 d. p. (3M)

3. Solve $x^4 - 5x^3 + 20x^2 - 40x + 60 = 0$ by Bairstow's method, starting with $p_0 = -4, q_0 = 8$. Perform two iterations and find the corresponding quadratic factor. (4M)

4. Solve by Gauss-Seidel method, correct to 3 d.p.:
$x + y + z = 9,\ 2x - 3y + 4z = 13,\ 3x + 4y + 5z = 40$ (3M)

5. Factorise A as LU where L is a lower triangular matrix and U is an upper triangular matrix:
$$\begin{pmatrix} 5 & -2 & 1 \\ 7 & 1 & -5 \\ 3 & 7 & 4 \end{pmatrix}$$ (3M)

6. Growth of bacteria (N) in a culture after t hours is given in the following table: Fit a curve of the form $N = a\,b^t$ for the data:

t	0	1	2	3	4	5	6
N	32	47	65	92	132	190	275

(4M)

7. Use Newton's divided difference formula to find $f(9)$:

x	5	7	11	13	17
f(x)	150	392	1452	2366	5202

(3M)

8. Evaluate $\int_4^{5.2} \log x\,dx$ by Simpson's $3/8$ rule. (3M)

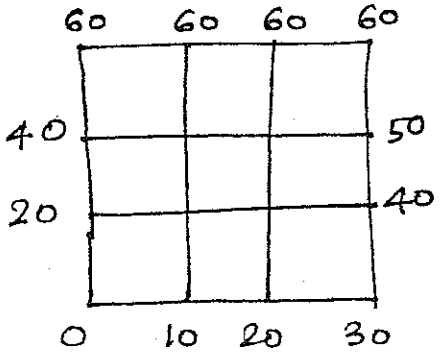
$y(0.3)$, $z(0.3)$

9. Solve $\frac{dy}{dx} = 1 + xz; \frac{dz}{dx} = -xy$ by R K method of order 4, given y=0, z=1 at x=0. (4M)

10. Solve $\frac{dy}{dt} = \frac{-2y}{t}$ by finding y at 4.5 with h = 0.5, given y(3.5) = 0.244898, y(4) = 0.1875, using non-self-starting Heun's method. (3M)

11. Solve $\frac{\partial^2 f}{\partial x^2} = \frac{\partial f}{\partial t}$ using Crank-Nicholson's scheme with h = 1 and k = 0.5 for one time step: $f(0;t) = f(5,t) = 0,\ f(x,0) = x^2(25 - x^2),\ 0 < x < 5$. (4M)

12. Solve the Laplace equation:



(3M)

All the Best!

BITS PILANI, DUBAI CAMPUS
DUBAI INTERNATIONAL ACADEMIC CITY, DUBAI

Second Year - Semester-II (2012-13)

COMPREHENSIVE EXAMINATION (Closed Book)

NUMERICAL METHODS FOR CHEMICAL ENGINEERS (CHE F242)

MARKING SCHEME

1. $f(\pi/3) = \cos(\pi/4) - \sin(\pi/4)\cdot(\pi/12) - \frac{1}{2}\cos(\pi/4)\cdot(\pi/12)^2$

$= 0.497754$ ——— (2M)

$E_t = 0.449\%$ ——— (1M)

2. Regular fabi formula ——— (1M)

The required root is

$x = 0.51775$ ——— (2M)

3. First iteration:

$p_1 = -3.8333$, $q_1 = 7.3333$ ——— (2M)

Second iteration:

$p_2 = -3.8333$, $q_2 = 7.3064$ ——— (2M)

$\therefore$ The corresponding quadratic factor

is $x^2 - 3.8333x + 7.3064$.

4. By Gauss-Seidel method:

$x = 1$, $y = 3$, $z = 5$ ——— (3M)

5. $L = \begin{bmatrix} 1 & 0 & 0 \\ 7/5 & 1 & 0 \\ 3/5 & 41/19 & 1 \end{bmatrix}$ $U = \begin{bmatrix} 5 & -2 & 1 \\ 0 & 19/5 & -32/5 \\ 0 & 0 & 327/15 \end{bmatrix}$

(1.5M) (1.5 M)

6. Given $N = ab^t$

$\Rightarrow \quad Y = A + Bt$ where

$Y = \log N, \quad A = \log a, \quad B = \log b$ —(½ M)

$\Rightarrow \quad a = 32.15, \quad b = 1.43$ —(1½ M)

$\therefore \quad N = 32.15\,(1.43)^t$ —(1½ M)

When $t = 7, \quad N = 387$ —(½ M)

7. <u>Divided diff. table:</u>

x	$f(x)$	Δf	$\Delta^2 f$	$\Delta^3 f$
5	150			
		121		
7	392		24	
		265		1
11	1452		32	
		457		1
13	2366		42	
		709		
17	5202			

—(1M)

$f(9) = y_0 + (x - x_0)\,[x_0, x_1] + (x - x_0)(x - x_1)\,[x_0, x_1, x_2] + \cdots$ —(3 M)

$= 810$

8. Simpson's 3/8 rule : formula — (½ M)

$$\int_{4}^{5.2} \log x \, dx = 1.827847$$ — (1M)

hints

x :	4	4.2	4.4	4.6	4.8	5.0	5.2
$\log x$:	1.3863	1.4351	1.4816	1.5261	1.5686	1.6094	1.6487

— (1½ M)

9. R.K. method : formula — (1M)

$y(0.3) = 0.3448$, $z(0.3) = 0.99$

— (3 M)

10. Formula : (predictor, corrector) — (1M)

$y_1^p = y_{-1} + 2h\, f(x_0, y_0)$

$= 0.151148$

$y_1^c = y_0 + \frac{h}{2}\left[f(x_0, y_0) + f(x_1, y_1^p)\right]$

$= 0.147268$

— (2M)

11. Crank Nicholson formula — (1 M)

$u_1 = \frac{u_2}{6} + 22 = 35.5$

$u_2 = 56 + \left(\frac{u_1 + u_3}{6}\right) = 81$

$u_3 = 86 + \left(\frac{u_2 + u_4}{6}\right) = 114.6$

$u_4 = 72 + \left(\frac{u_3}{6}\right) = 91.1$

— (3 M)

12. $u_1 = 26.66$

$u_2 = 33.33$

$u_3 = 43.33$

$u_4 = 46.66$

(3M)

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SECOND SEMESTER 2012-13
CHE F242 NUMERICAL METHODS FOR CHEMICAL ENGINEERS
Test 2 (Open Book)

Weightage: 20% | Date: 02.05.2013
Max. Marks: 20 | Time: 11.10 AM -12.00 Noon

Answer all the questions.
No programmable calculators are allowed.
Only Text book and Hand written Class notes are allowed.

1. Using LU decomposition method, solve $3x+2y+7z=4,\ 2x+3y+z=5,\ 3x+4y+z=7$ (5M)

2. Fit a curve of the form $y = a\,x^b$ for the data:

x	1	2	3	4	5
y	7.1	27.8	62.1	110	161

(5M)

3. Obtain a natural cubic spline for the data in the interval $[2, 3]$ and find *y* at *x* = *2.5*

x	0	1	2	3
y	1	2	33	244

(5M)

4. Find the area under the curve between *x=1* and *x=4* by Simpson's $3/8$ rule:

x	1	1.5	2	2.5	3	3.5	4
y	2	2.4	2.7	2.8	3	2.6	2.1

(5M)

All the Best!

BITS PILANI, DUBAI CAMPUS
Dubai International Academic City, Dubai
Second Semester 2012-13

CHE F242 Numerical Methods for Chemical Engineers
Test 2 (Open Book)

MARKING SCHEME

1. $A = \begin{bmatrix} 3 & 2 & 7 \\ 2 & 3 & 1 \\ 3 & 4 & 1 \end{bmatrix}$

$L = \begin{bmatrix} 1 & 0 & 0 \\ 2/3 & 1 & 0 \\ 1 & 6/5 & 1 \end{bmatrix}$ ——— (2M)

$U = \begin{bmatrix} 3 & 2 & 7 \\ 0 & 5/3 & -11/3 \\ 0 & 0 & -8/5 \end{bmatrix}$ ——— (2M)

The solution set is $\{ 7/8, 9/8, -1/8 \}$ —(1M)

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2. Taking log. on bothsides,

$\log y = \log k + m \log x$

$\Rightarrow \quad Y = A + mX \longrightarrow (1)$ ——— (1M)

where $Y = \log y$, $X = \log x$

Forming the table and solving for the unknowns, we get ——— (2M)

$k = 7.17$, $m = 1.95$ ——— (2M)

$\therefore$ the required curve is

$y = 7.17\, x^{1.95}$

3. Let the cubic spline be

$$y = a_i (x - x_i)^3 + b_i (x - x_i)^2 + c_i (x - x_i) + d_i, \quad i = 0, 1, 2$$

Here $S_3 = 0 = S_0$

$$\begin{bmatrix} 2(h_0 + h_1) & h_1 \\ h_1 & 2(h_1 + h_2) \end{bmatrix} \begin{bmatrix} S_1 \\ S_2 \end{bmatrix} = 6 \begin{bmatrix} \Delta f_1 - \Delta f_0 \\ \Delta f_2 - \Delta f_1 \end{bmatrix}$$

$$\Rightarrow \begin{pmatrix} 4 & 1 \\ 1 & 4 \end{pmatrix} \begin{pmatrix} S_1 \\ S_2 \end{pmatrix} = \begin{pmatrix} 180 \\ 1080 \end{pmatrix} \quad \text{——— (2M)}$$

Solving $S_1 = -24$, $S_2 = 276$ ——— (1½M)

when $2 \le x \le 3$,

$a_2 = -46$, $b_2 = 138$, $c_2 = 119$, $d_2 = 33$. ——— (1M)

$$\therefore y = -46 (x-2)^3 + 138 (x-2)^2 + 119 (x-2) + 33, \quad 2 \le x \le 3. \quad \text{——— (1M)}$$

$y(2.5) = 121.25$ ——— (½M)

4. By Simpson's ⅓ rule:

$$\int = \frac{h}{3} (A + 4B + 2C) \quad \text{——— (1M)}$$

$$= 7.7833 \quad \text{——— (2M)}$$

$(A = 4.1, \quad B = 7.8, \quad C = 5.7)$ ——— (2M)

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BITS PILANI, DUBAI CAMPUS
DUBAI INTERNATIONAL ACADEMIC CITY, DUBAI

SECOND SEMESTER 2012-13
CHE F242 NUMERICAL METHODS FOR CHEMICAL ENGINEERS
Test 1 (Closed Book)

Weightage: 25% | Date: 14.03.2013
Max. Marks: 25 | Time: 11.10 AM -12.00 Noon

Answer all the questions.
No programmable calculators are allowed.

1. Use the first and third order Taylor Series to predict the function at 1.2 with the base point $x = 1$ where $f(x) = 25x^3 - 6x^2 + 7x - 88$. Also compute the true relative percent error. (6M)

2. Find a real root of $x^3 - 5x + 3 = 0$ by the secant's method which lies between 1 and 2 by performing four iterations. (6M)

3. Find a real root of $x^3 - 2x - 5 = 0$ by the regula-falsi formula correct to 3 d.p. (6M)

4. Use the modified Newton-Raphson method to find a real root of $x^3 - 5x^2 + 7x - 3 = 0$ correct to 4 d.p. with initial guess $x_0 = 0$. Also compute the true relative percent error. (7M)

All the Best!

BITS PILANI, DUBAI CAMPUS

Dubai International Academic City, Dubai

Second Semester 2012-13

CHE F242 Numerical Methods for Chemical Engineers

Test 1 (Closed Book)

MARKING SCHEME

Q. no (1)

$$f(x) = 25x^3 - 6x^2 + 7x - 88$$
$$f'(x) = 75x^2 - 12x + 7$$
$$f''(x) = 150x - 12$$
$$f'''(x) = 150$$

(1M)

First order approximation:

$f(1.2) = -48$

True value $= -45.04$

Relative percent Error $\simeq 6.57\%$

(2.5M)

Third order approximation:

$f(1.2) = -45.04$

Relative percent error $\simeq 0\%$

(2.5 M)

Q. no (2)

Secant's formula — (1M)

$x_1 = 1.5$, $x_2 = 1.764759$,

$x_3 = 1.8735976$, $x_4 = 1.8312058$

(5M)

Q. No. 3

Regula-fabi formula — (1M)

The reqd. root is 2.093 — (5M)

Q. No 4

Modified NR formula — (1M)

x	E_t
$x_1 = 1.105263$	10.5263 %
$x_2 = 1.003082$	0.3082 %
$x_3 = 1.000002$	0.0002 %

(4 + 2 M)

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