UPES

UNIVERSITY OF PETROLEUM AND ENERGY STUDIES

End Semester Examination, December 2017

Program:	B. Tech. Chemical Engg. (spl. RP); CE-RP	Semester:	V
Subject (Course):	Numerical Methods in Chemical Engineering	Max. Marks:	100
Course Code:	MATH 311	Duration:	3 Hrs
No. of page/s:	0 + 3		

In this <u>OPEN BOOK and NOTES EXAM</u>, you are allowed to have the textbook (S. K. Gupta, *Numerical Methods for Engineers*), *all* handouts provided, *your own class-notes* and your solutions to assignment problems

- 1. Show all *intermediate steps* of your answers (and not just the final answers) to earn marks
- 2. *Please answer the questions in the sequence:* 1, 2, 3. You can do this by assigning, *a priori*, a few pages to each question, in the correct sequence. You may then answer the questions in whatever sequence you wish to, *all parts in one place*
- 3. No student is allowed to leave the examination hall in the first hour of the exam

Section A: XXX No questions here

Section B: ALL THREE QUESTIONS ARE COMPULSORY [Total 100 Marks]

Q.1 Consider the following set of coupled, non-linear ODE-BVPs with a single independent variable, *x*, and **two** dependent variables, y(x) and z(x), with $0 \le x \le 1$, $0 \le y \le 1$, $0 \le z \le 1$:

 $y'' + 3y = 3y^2z$

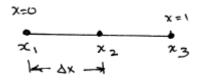
 $z'' + 4z = 2y + 6z^2$

with the following BCs:

Continued...

- y'(0) = 5; y(1) = 4
- z(0) = 2; z(1) = 6

(i) Use N = 2 (i.e., N + 1 = 3) and the FD method with expressions correct to $O(\Delta x)^2$ to solve this problem (give the *complete* set of equations) (30)



(30 Points)

(09)

(09)

(09)

Q.2 Consider the explicit, third order Hermite ODE-IVP algorithm (given in Table 5.1):

$$y_{n+1} = -4y_n + 5y_{n-1} + h(4y'_n + 2y'_{n-1}) + O(h^3)$$

(a) Obtain the characteristic equation for this technique.

(b) Obtain <u>*all*</u> the roots, μ_i , of this equation.

(c) Identify which of these roots is the non-spurious root, μ_1 .

Hint: You may use the following expansions:

$$(1+x)^{\frac{1}{2}} = 1 + \frac{1}{2}x - \dots$$
, and
 $e^{x} = 1 + x \dots$

(d) Now evaluate the numerical value of $|\mu_1|$ for $|h\lambda| = 0$ (08) (35Points)

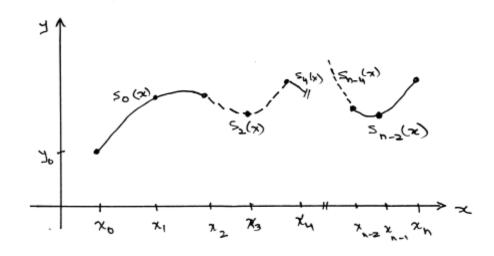
Q.3 Consider a <u>NEW quadratic</u> spline fit for a set of given points, (x_0, y_0) , (x_1, y_1) , (x_2, y_2) , ..., (x_n, y_n) , with *n* being an <u>even number</u>. You decide to fit <u>each</u> of the quadratic splines to three adjacent points as follows (see diagram below):

Continued...

 $S_0(x)$: Points (x_0, y_0) , (x_1, y_1) and (x_2, y_2) ,

 $S_2(x)$: Points (x_2, y_2) , (x_3, y_3) and (x_4, y_4) , ...

 $S_{n-2}(x)$: Points (x_{n-2}, y_{n-2}) , (x_{n-1}, y_{n-1}) and (x_n, y_n) .



Note again that each of the spines are quadratic (*not linear nor cubic*) and each passes through three points as discussed above (this is a stupid thing to do, but you still do it).

- (a) Write down the <u>most convenient</u> equations for $S_i(x)$, i = 0, 2, 4, ..., n 4, n 2, involving constants, $a_{i,i}$. (10)
- (b) Write down *all* the equations for determining the constants, a_{i,j}. Since the algebra involved is quite a bit, do *not* solve these equations (except the ones which are extremely simple).
 (12)
- (c) Comment on the continuity of the *values* of $S_i(x)$ and $S_{i+2}(x)$ at the end-points, i.e., at $x = x_{i+2}$, as well as the values of $S'_i(x)$ and $S''_i(x)$ at these points. (13) (35 Points)