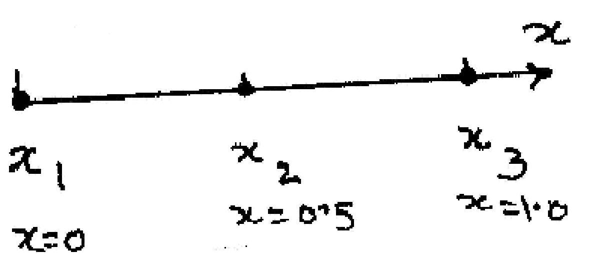
Name: **Enrolment No:**	UPES

UNIVERSITY OF PETROLEUM AND ENERGY STUDIES

End Semester Examination, December 2018

Course: Numerical Methods in Chemical Engineering
Semester: V

Programme: B. Tech. CE-RP (Chemical Engineering-RP)
Time: 03 hrs. **Max. Marks: 100**
Instructions: **Open Books and Notes, etc.**
Question Paper has to be returned at the end of the exam

	SECTION A		
S. No.		**Marks**	**CO**
Q 1	Statement of question **NIL (open book exam)**	**x**	**CO1**
	SECTION B		
Q	Statement of question **NIL (open book exam)**	**x**	**CO4**
	SECTION-C: ALL THREE QUESTIONS ARE COMPULSORY (Total 100 Marks)		
Q1	Consider the following ODE-BVP: $$\frac{d^2y}{dx^2}+2yx=xy\int_{x=0}^{1}\left(y^2e^x\right)dx;\ 0\le x\le 1$$  with $y(x=0)=2$;		**CO5**

and $y(x = 1) = 6$

Use $N = 2$ (therefore, $N + 1 = 3$ FD points, x_1, x_2 and x_3)

(a) Write the values of y_1 and y_3 (05)

(b) Use Simpson's rule (with $h = 0.5$) to evaluate the integral on the right hand side. Compute all the values and give a simple ***final*** expression (10)

(c) Use the finite difference technique to obtain an equation for y_2. Simplify as much as possible (10)

(d) Check if $y_2 = 0.345$ satisfies this equation (05)

(***30 Points***)

Q2 Consider the following ODE-IVP involving two variables, y_1(t) and y_2(t):

¿

with $\boldsymbol{y}(t = 0) = \boldsymbol{y}_0 = [2 \quad 1]^T$

(a) Apply the ***implicit*** Euler technique (for one step only, i.e., from $t = 0$ to $t = h = 0.1$) to obtain your answers in the following form:

$F(y) \equiv$ ¿ (10)

(b) Now use the Newton-Raphson-Kantarovich technique ***WITHOUT*** using inverses in any part of this question to obtain

¿

Do ***one*** NRK iteration only. Obtain ***numerical*** answers (10)

(c) Plug in your answers in part (b) of this question (i.e., into the $\boldsymbol{F}(\boldsymbol{y}) = \boldsymbol{0}$ equation) and see what you get (05)

(d) Comment on your answer to part (c) of this question. (10)

	(***35 Points***) ***Continued . .***		
Q3	Consider the third order ($q - 1 = 3$) implicit Hermite algorithm (in Table 5.1) of integrating ODE-IVPs for a single variable, $y(x)$, with $\alpha_0 = \frac{1}{2}$ $\alpha_1 = \alpha_3 = \alpha_4 = \ldots = 0$ $\alpha_2 = \frac{1}{2}$ $\beta_0 = \frac{-1}{4}$ $\beta_1 = \beta_3 = \beta_4 = \ldots = 0$ $\beta_2 = \frac{1}{4}$ (a) Write down the algorithm for y_{n+1} in terms of y_i and y_i' (05) (b) Using $\frac{dy}{dt} = \lambda y$, $y(t=0) = y_0$, obtain the characteristic equation for μ and solve for μ_i [Hint: Note that you will get ***two*** values of μ_i] (10) (c) Which of these two roots is the ***genuine*** root and which is the ***spurious*** root (05) (d) What is the ***requirement of stability*** for this problem. (15) (***35 Points***) * * *		