Name: **Enrolment No:**	UPES UNIVERSITY WITH A PURPOSE

UNIVERSITY OF PETROLEUM AND ENERGY STUDIES
End Semester Examination, Dec 2021

Course: Chemical Engineering Computing **Semester: I**
Program: M. Tech (Chemical Engineering) **Time: 3 hrs**
Course Code: CHPD 7002 **Max. Marks: 100**

Instructions: (1) Answer **ALL** questions
(2) Assume the appropriate value of missing data, if any.

SECTION A (20 M)

S. No.		**Marks**	**CO**
Q1	Why LU decomposition is better than Gauss Elimination method for solving the system of linear equations in specific case ?	**4**	**CO1**
Q2	Suppose we are in the three dimensional space, and the three planes in the row picture do not intersect at a common point of intersection. What are the various possibilities for the infinite solutions and no solution. Demonstrate with the help of suitable examples of the equation of planes.	**4**	**CO1**
Q3	What is the criterion of convergence for the Gauss Elimination and LU decomposition method ?	**4**	**CO2**
Q4	What is the criterion of convergence for the the fixed point iteration method for system of non-linear equations ?	**4**	**CO2**
Q5	Write the names of two open methods to solve non-linear equation. Compare and contrast the two methods in terms of their convergence.	**4**	**CO1**

SECTION B (50 M)

Q6	It is known that the root of the equation $\cos x = xe^{x}$ lie in the interval (0, 1). Estimate the the value of x with an accuracy of 0.05 using bisection method.	**10**	**CO3**
Q7	Using finite difference (central difference in space) method to solve the differential equation $\frac{d^2y}{dx^2} - 2y = x^2 - 2x - 4, \quad 0 < x < 1$	**10**	**CO3**

With the Dirichlet boundary conditions

At $x = 0$, $y = 0$
At $x = 1$, $y = -1$

If x = 1 m. Take $\Delta x = 1/3$ to find the values of y at all nodes.

Q8 (**10**, **CO3**)

Draw the column picture (Linear combination) for the system of linear equations, Ax = b.

$$\text{Where } A = \begin{bmatrix} 1 & 10 & -1 \\ 2 & 3 & 20 \\ 10 & -1 & 2 \end{bmatrix}, \ b = \begin{bmatrix} 3 \\ 7 \\ 4 \end{bmatrix} \text{ and } x = \begin{bmatrix} x & y & z \end{bmatrix}^T$$

Do the linear combinations of these column fill the entire 3D-space? Solve them using LU decomposition method.

OR

Solve the system of Non-linear equations by Newton Raphson Method.

$$f_1(x_1, x_2) = 3x_1^3 + 4x_2^2 - 145 = 0$$
$$f_2(x_1, x_2) = 4x_1^2 - x_2^3 + 28 = 0$$

Q9 (**10**, **CO3**)

Fit a second order polynomial using least square method to the following data

x	0	1	2	3	4	5
y	2.1	7.7	13.6	27.2	40.9	61.1

SECTION C (40 M)

Q10 (**20**, **CO4**)

Consider a series reaction $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ carried out in a batch reactor. The differential equation for component A is,

$$\frac{dC_A}{dt} = -k_1 C_A$$

for component B is,

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B$$

and for component C ,

	$$\frac{dC_c}{dt} = k_2 C_B$$ The initial condition is: at t =0, $C_A = 1, C_B = 0,$ and $C_c = 0$. The rate constants are $k_1 = k_2 = 1$ sec^{-1}. Use the fourth order Runge - Kutta method to determine the concentration of A, B and C up to 4 sec, using step size of 2 sec.		
Q11	A fin of diameter 0.02 m and length 0.05 m is attached to a wall. The temperature of the wall is 320 ^oC. The thermal conductivity of the fin material and the heat transfer coefficient from the fin to the surrounding are 50 W/m-K and 100 W/m^2-K. The temperature of the surrounding is 20 ^oC. The governing equation is $-\frac{d^2\theta}{dx^2} + \frac{hP}{kA}\theta = 0,$ where $\theta = T - T_{surr}$, P is the perimeter and A is the area of cross section of the fin. The boundary condition at x = 0.05 m is $\frac{d\theta}{dx} + \frac{h}{k}\theta = 0$. Formulate the problem into the system of linear equation to find the temperature of the fin at x = 0.0124, 0.025, 0.0375 and 0.05. You are not required to obtain the solution.	**20**	**CO4**