Name: Enrolment No:	

UPES
End Semester Examination, June 2025

Course: Introduction to Computational Physics **Semester : II**
Program: M. Sc. Physics **Time : 03 hrs.**
Course Code: PHYS7031 **Max. Marks: 100**

Instructions:
1. **All questions are compulsory.**
2. **Question 7 in section B has an internal choice.**
3. **Question 10 in section C has an internal choice.**
4. **Use of scientific calculators is allowed.**
5. **Number of Pages: 3.**

SECTION A
(5 Q x 4 Marks = 20 Marks)

S. No.		Marks	CO
1	Define truncation and round-off errors. Give one numerical example of each.	**4**	**CO1**
2	Create a flowchart for calculating the sum of the digits of a given integer.	**4**	**CO1**
3	Develop a Gnuplot script to plot a histogram of a dataset stored in a text file.	**4**	**CO3**
4	Write a C++/FORTRAN code snippet to swap two numbers using a function/subroutine.	**4**	**CO2**
5	Compose a LaTeX code snippet to display the following expression in display mode: $$V(r) = \frac{1}{4\pi\epsilon_0}\sum_{i=1}^{n}\frac{q_i}{\sqrt{(x-x_i)^2}}$$ Format the equation using appropriate LaTeX syntax for summation, fractions, and square roots. Clearly define each symbol.	**4**	**CO3**

SECTION B **(4 Q x 10 Marks = 40 Marks)**			
6	Develop a LaTeX document (preamble + body) for a lab report that includes a title, a table, and an equation section.	**10**	**CO3**
7	Describe how curve fitting is done using Gnuplot. Use the following data to fit a quadratic model: x: 1, 2, 3, 4, 5; y: 2.1, 4.2, 7.8, 13.5, 21.2. Write the Gnuplot script to fit the function of form $y = ax^2 + bx + c$. Include the fit process, parameter values, residual analysis, and a plot overlaying the data and fitted curve. What is the goodness of fit? ***OR*** Write Gnuplot commands to Generate a contour plot and 3D surface of $z = e^{-(x^2+y^2)}$ using Gnuplot. Explain each line of the script.	**10** **10**	**CO3** **CO3**
8	Applying the Trapezoidal Rule, evaluate the integral $\int_1^3 ln(x)\ \text{dx}$ using 4 subintervals. Show all steps.	**10**	**CO4**
9	Compute the derivative of $f(x) = \sin(x)$ at $x = \frac{\pi}{4}$ using the forward difference method with step size $h = 0.01$. Display the result and compare it with the analytical derivative $f'(x) = \cos(x)$.	**10**	**CO4**
SECTION-C **(2 Q x 20 Marks = 40 Marks)**			
10	Evaluate the following initial value problem using the 4th Order Runge-Kutta Method:	**20**	**CO4**

	$\frac{dy}{dx} = y - x^2 + 1,$ with $y(0) = 0.5$, find $y(0.2)$ using step size $h = 0.1$. ***OR*** Use Lagrange Interpolation to find $f(2.5)$ from the following data: x: $1, 2, 3$ $f(x)$: $1, 4, 9$		
11	Explain the Newton-Raphson Method and compare it with the Secant Method. Use the Newton-Raphson method to find the root of $f(x) = x^3 - 2x - 5$ with initial guess $x_0 = 2$, up to 3 decimal places.	**20**	**CO4**