Name: **Enrolment No:**	UPES UNIVERSITY OF TOMORROW

UPES

End Semester Examination, May 2025

Course: Numerical Methods in Scientific Computing | **Semester: VI**

Program: BSc (H) Physics | **Time : 03 hrs.**

Course Code: PHYS 3026P | **Max. Marks: 100**

Instructions:

SECTION A

(5Qx4M=20Marks)

S. No.		Marks	CO
Q1	Differentiate between explicit and implicit schemes in numerically approximating time-dependent ODEs?	**4**	**CO1**
Q2	Describe the different types of boundary conditions used in solving partial differential equations (PDEs).	**4**	**CO1**
Q3	Compare direct and iterative methods of solving a system of linear equations. Explain which method should, in principle, provide the best accuracy if properly implemented and why?	**4**	**CO2**
Q4	For the following system of non-linear equations, derive a form of the Jacobian matrix considering $(x_1^{(1)}, x_2^{(1)}, x_3^{(1)})^t = (-1,2,1)^t$: $$-2x_2^2 + x_2 - 2x_3 - 5 = 0$$ $$8x_2^2 + 4x_3^2 - 9 = 0$$ $$8x_2x_3 + 4 = 0$$	**4**	**CO1**
Q5	How is Lagrange interpolation different from cubic spline interpolation? Explain briefly.	**4**	**CO1**

SECTION B

(4Qx10M= 40 Marks)

Q6	Approximate the following function using Lagrange Interpolating polynomials $$f(x) = \cos x + \sin x$$ using $x_0 = 0, x_1 = 0.25, x_2 = 0.5, x_3 = 1.0$ nodes. Also, find the upper bound on the error. **OR** Construct an interpolating polynomial using Newton's divided difference method with the help of the following data: <table><tr><th>x</th><th>$f(x)$</th></tr><tr><td>-0.1</td><td>5.30000</td></tr></table>	**10**	**CO3**

<table>
<tr>
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0.0	2.00000
0.2	3.19000
0.3	1.00000

If the approximated function is $P(x)$, find $P(0.35)$.
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<td>Q7</td>
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Using composite trapezoidal rule, approximate the following integral:

$$\int_0^{\pi/4} e^{3x} \sin 2x \; dx$$

Also, estimate the error in the integration.

Composite trapezoidal rule is given as:

$$\int_a^b f(x)dx \approx \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{(b-a)}{12} h^2 f^{(2)}(\mu)$$
</td>
<td>10</td>
<td>CO4</td>
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<td>Q8</td>
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At a time $t = 0$, a tank contains Q_0 lb (1 lb = 0.45 Kg) of salt dissolved in 100 gal (1 gallon = 3.785 liter) of water (see the figure). Assume that water containing 1/4 lb of salt/gal is entering the tank at a rate of r gal/min, and that the well-stirred mixture is draining from the tank at the same rate. This flow process is represented by the following ODE:

$$\frac{dQ}{dt} + \frac{rQ}{100} = \frac{r}{4}$$

where $Q(t)$ is the amount of salt in the tank at a time t. If $r = 3$ and $Q_0 = 75$ lb, find the time T after which the salt level is 6% of Q_0. Also, find the flow rate that is required if the value of T is not to exceed 4 min. Use RK2 method for the numerical solution. Choose the discretization details (e.g. time step, Δt) as needed.

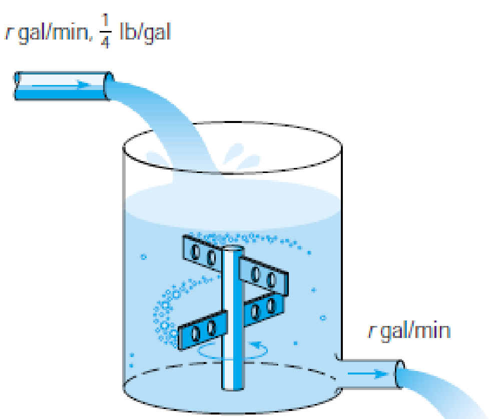

Figure: Water tank in question 8
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<td>10</td>
<td>CO4</td>
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	The RK2 /Heun's method is given as: $$y_{kp} = y_k + hf(t_k, y_k)$$ $$y_{k+1} = y_k + \frac{h}{2}\left[f(t_k, y_k) + f(t_k + h, y_{kp})\right]$$		
Q9	Use Newton's method to find 3 iterates ($\boldsymbol{x}^{(3)}$) of the following system of non-linear equations: $$15x_1 + x_2^2 - 4x_3 = 13$$ $$x_1^2 + 10x_2 - x_3 = 11$$ $$x_3^2 - 15x_3 = -22$$ Also calculate $\left\|\boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)}\right\|_\infty$ to see convergence to the solution. Consider the accuracy as 10^{-4}. Use the guess vector as $\boldsymbol{x}^{(0)} = (0,0,0)^t$.	**10**	**CO2**
SECTION-C **(2Qx20M=40 Marks)**			
Q10	(**a**) Using 3- step Adam's Bashforth method to solve the following ODE: $$\frac{dy}{dt} = \cos 2t + \sin 3t, \quad 0 \le t \le 1, \qquad y(0) = 1 \text{ with } h = 0.25$$ 3-step Adam's Bashforth method is given as: $$y_{j+1} = y_j + \frac{h}{12}\left[23f(t_j, y_j) - 16f(t_{j-1}, y_{j-1}) + 5f(t_{j-2}, y_{j-2})\right] + \frac{3}{8}f^{(3)}(\mu_j)h^3$$ (**b**) The air pressure $p(x,t)$ in an organ pipe is governed by the wave equation $$\frac{\partial^2 p}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 p}{\partial t^2}, \quad 0 < x < l, 0 < t$$ where l is the length of the pipe, and c is a physical constant. If the pipe is open, the boundary conditions are given by $$p(0,t) = 0.9 \text{ and } \frac{\partial p}{\partial t}(l,t) = 0$$ Assume $c = 1, l = 1$, and the initial conditions are $$p(x,0) = 0.9\ \cos 2\pi x \quad \text{and} \quad \frac{\partial p}{\partial t}(x,0) = 0, \quad 0 \le x \le 1$$	**10 + 10**	**CO4**

	Take $h = 0.25$ and $k = 0.1$. Discretize both the differential operators using centered differencing and then express the system of discretized equations in $Ap = b$ form. **OR** (**a**) Using RK4 method, solve the following ODE: $\frac{dy}{dt} = 1 + (t - y)^2, \quad 2 \le t \le 3, \quad y(2) = 1$ Take $h = 0.2$. The RK4 method is given as: $y_{k+1} = y_k + \frac{h}{6}[K_1 + 2K_2 + 2K_3 + K_4]$ $K_1 = f(t_k, y_k)$ $K_2 = f\left(t_k + \frac{h}{2}, y_k + \frac{h}{2}K_1\right)$ $K_3 = f\left(t_k + \frac{h}{2}, y_k + \frac{h}{2}K_2\right)$ $K_4 = f(t_k + h, y_k + hK_3)$ (**b**) Using finite difference method discretize the Laplace equation given below: $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \qquad 1 < x < 2, \quad 0 < y < 1$ $u(x,0) = 2\ln x, \quad u(x,1) = \ln(x^2+1), \quad 1 \le x \le 2$ $u(1,y) = \ln(y^2+1), \quad u(2,y) = \ln(y^2+4), \quad 0 \le y \le 1$ Use $h = k = \frac{1}{3}$. Write the discretized equations in terms of $A\boldsymbol{u} = \boldsymbol{b}$, where A is the coefficient matrix, $\boldsymbol{u}$ is the unknown and $\boldsymbol{b}$ is known vector.		
Q11	The temperature $u(x,t)$ of a long, thin rod of constant cross section and homogeneous conducting material is governed by 1-D heat equation. If heat is generated in the material, for example, by resistance to current or nuclear reaction, the heat equation becomes: $\frac{\partial^2 u}{\partial x^2} + \frac{Kr}{\rho C} = K\frac{\partial u}{\partial t}, \quad 0 < x < l, \ 0 < t$ where l is the length, ρ is the density, C is the specific heat, and K is the thermal diffusivity of the rod. The function $r = r(x,t,u)$ represents the heat generated per unit volume. Suppose that	**20**	**CO4**

	$l = 1.5$ cm, $K = 1.04$ cal/cm-deg-sec, $\rho = 10.6$ g/cm^3, $C = 0.056$ cal/g-deg and $r(x,t,u) = 5.0$ cal/cm^3-s If the ends of the rod are kept at 0°C, then $$uc(0,t) = u(l,t) = 0, \quad t > 0$$ Suppose the initial temperature distribution is given by $$u(x,0) = \alpha_0, \quad 0 \le x \le l$$ Using $h = 0.15$ (space discretization step) and $k = 0.0225$ (time discretization step), discretize the above PDE by approximating the time derivative using the implicit Euler and the spatial derivative using the centered differencing. Write the discretized equations in the form of $Au = b$ and discuss the solution strategy.		