No. of Printed Pages : 3 **RPHI–002**

M. SC. (PHYSICS) (MSCPH)

Term-End Examination

June, 2026

RPHI-002 : COMPUTATIONAL TECHNIQUES

Time : $1\frac{1}{2}$ Hours *Maximum Marks : 25*

Note : *(i) All questions are compulsory. However, internal choices are given.*

(ii) Symbols have their usual meanings.

(iii) You may use a calculator.

1. Answer any *three* parts : 3×5=15

(a) Explain round off error and truncation error. If the function e^x is written as :

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!}$$

determine the truncation error in calculating $e^{1.5x}$ at $x = 2$. 2+3

(b) Write the forward difference approximation, backward differences approximation and central difference approximation for calculating the first order derivative of a continuous function $f(x)$. Derive the order of accuracy in the approximate value of the derivative in each case. 2+3

(c) Use the multiple segment Simpson's rule with 4 segments to evaluate the integral : 5

$$\int_0^3 \frac{1}{1+x^5}$$

(d) Fit the data given in the table below to the exponential model $y = \mathrm{A}\, e^{bt}$: 5

t	y
0	1
1	0.9
3	0.7
5	0.55
7	0.45

(e) Explain the central idea behind Density functional theory. What is the Kohn-Sham method ? 2+3

2. Answer any *one* part : 1×10=10

(a) Solve the following set of equations using the method of LU decomposition :

$$2x + y - z = 1$$
$$x + 2y + z = 8$$
$$-x + y - z = -5$$

(b) (i) Solve the following second order ordinary differential equation using Euler's method to obtain the value of y at $x = 3$:

$$y'' = x^2 + y^2 + y'$$

Use the initial conditions $y(0) = 4$, $y'(0) = 3$ and the value of $h = 3$.

(ii) Describe one numerical method that improves upon the accuracy of the Euler's method of solving ODEs. 6+4

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