

SHRIMATHI DEVKUNVAR NANALAL BHATT VAISHNAV COLLEGE FOR WOMEN
(AUTONOMOUS)

(Affiliated to the University of Madras and Re-accredited with 'A+' Grade by NAAC)

Chromepet, Chennai — 600 044.

M.Sc.(Physics) END SEMESTER EXAMINATIONS APRIL - 2023

SEMESTER - II

22PPHCT2007 - Computational Methods and C Programming

Total Duration : 2 Hrs. 30 Mins.

Total Marks : 60

Section B

Answer any **SIX** questions ($6 \times 5 = 30$ Marks)

1. If $y(75) = 246$, $y(80) = 202$, $y(85) = 118$, $y(90) = 40$ find $y(79)$.
2. Use Lagrange's formula to find the value of y at $x = 6$ from the following data:

x	3	7	9	10
y	168	120	72	63

3. Prove that every square matrix and its transpose have the same eigen values.
4. Solve the following simultaneous equations to second approximation using Jacobi's method.

$$20x + y - 2z = 17$$

$$3x + 20y - z = -18$$

$$2x - 3y + 20z = 25$$
5. Write a C program to find the real root of a given equation using bisection method.

6. Evaluate using trapezoidal rule considering five subintervals. $\int_0^1 \frac{1}{1+x} dx$
7. Arrive at Simpson's three-eighth rule from Newton-Cote's quadrature formula.
8. Describe on Born Oppenheimer approximation.

Section C

I - Answer any **TWO** questions ($2 \times 10 = 20$ Marks)

9. Write a C program to find out the value of y for a corresponding value of x using Lagrange's interpolation if a data set is given as the input
10. Solve the following system of equations using Gauss elimination method:

$$28x + 4y - z = 32$$

$$x + 3y + 10z = 24$$

$$2x + 17y + 4z = 35$$

Contd...

11. Write a C program to compute the solution of the initial value problem using fourth order Runge - Kutta method for the function $xy + y^2$.
12. Discuss in detail on the theories on exchange correlation functions.

II - Compulsory question ($1 \times 10 = 10$ Marks)

13. Find the root of the equation $\sin x = 1 + x^3$ between $(-2, -1)$ to 3 decimal places by Newton - Raphson method.

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