

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 2025

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. Derive Newton's forward difference formula.
2. Explain the algorithm for the Newton-Raphson method in solving transcendental equations.
3. Evaluate $\int_{-3}^3 x^4 dx$ by using
(i) Trapezoidal rule (ii) Simpson's one-third rule.
4. Compare Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA) in DFT.
5. Apply Power Method for finding eigen values of a matrix.
6. Find the positive root of $f(x) = 2x^3 - 3x - 6 = 0$ by Newton-Raphson method correct to five decimal places.
7. Compute one iteration of the Modified Euler's Method for $dy/dx = x + y$ with $y(0) = 1$ and $h = 0.2$.
8. How does the Kohn-Sham equation differ from the Schrödinger equation?

Section C

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

9. Write a C programme for Lagrange Interpolation with step-by-step algorithm.
10. Using Gauss Elimination method, Solve the system:
 $3.15x - 1.96y + 3.85z = 12.95.$
 $2.13x + 5.12y - 2.89z = -8.61.$
 $5.92x + 3.05y + 2.15z = 6.88.$
11. Write a C program to solve a transcendental equation using the Bisection method. Explain the logic and provide sample output.

Contd...

12. Implement a C program to compute the Runge-Kutta 2nd order method for solving first-order differential equations.

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

13. Derive and explain the Born-Oppenheimer approximation and discuss its impact on molecular structure calculations.
