M.Sc. PHYSICS SEMESTER - III

CORE X - COMPUTATIONAL METHODS AND PROGRAMMING

UNIT I: C++ programming

Constants, variables and their declarations – Input, output and comparison operators–if, if. else, switch, while, do-while, for, break statements – main, void, exit, swap functions – Arrays – passing by value and passing by reference.

UNIT II: Curve fitting and interpolation

Curve fitting: Method of least squares – Normal equations – Straight line fit – Exponential and power – law fits. Newton interpolation polynomial: Linear Interpolation – Higher order polynomials – First- order divided differences – Gregory - Newton interpolation polynomials-Lagrange interpolation – Truncation error.

UNIT III: Solutions of Linear and Nonlinear Equations

Simultaneous linear equations: Gauss elimination method – Jordan's modification – Inverse of a matrix by Gauss- Jordon Method – Roots of nonlinear equations: Newton-Raphson method – Iterative rule – Termination criteria – Pitfalls – Order of convergence

UNIT IV: Numerical integration and Differentiation

Newton-Cotes quadrate formula – Trapezoidal, Simpson's 1/3 and 3/8 rules – Errors in the formulas. Differentiation: First –order derivative:-Two and four-point formulas second –order derivative: Three and five-point formulas.

UNIT V: Numerical solution to ordinary Differential Equations

First-order equations: Euler and improved Euler methods – Formulas – Local and global truncation errors – Fourth-order Runge-Kutta method – Geometric description of the formula– Errors versus step size –Second order equation – Euler methods and Fourth order Runge -Kutta method.