M.Sc Physics Semester - III Paper XX
Computational Physics – I 23PHY23DB1

Theory Marks:80
Internal Assessment Marks:20
Time: 3 Hours

COURSE OUTCOMES

CO1 Students would acquire a vision for use of computer inresearch prospective.
CO2 Students would be able to recognize the nature of a specific numerical problem and would develop the acumen for choosing an appropriate numerical technique to find its solution.
CO3 Students would be able to design Fortran programs to solve numerical computationally.

Unit I

Numerical Integration: Newton-cotes formulae: Trapezoidal rule, Simpson's 1/3 rule, error estimates in Trapezoidal rule and Simpson 1/3 rule using Richardson deferred limit approach; Gauss-Legendre quadrature method; Monte Carlo (mean sampling) method for single, double and triple integrals. Numerical Differentiation: Taylor Series method; Generalized numerical differentiation: truncation errors. Roots of Linear, Non-linear Algebraic and Transcendental equations: Newton-Raphson method; convergence of solutions. Curve Fitting: Principle of least square; Linear regression; Polynomial regression; Exponential and Geometric regression.

Unit II

Interpolation: Finite differences; Interpolation with equally spaced points; Gregory - Newton's Interpolation formula for forward and backward interpolation; Interpolation with unequally spaced points:Lagrangian interpolation, Solution of Simultaneous Linear Equations: Gaussian elimination method, Pivoting; Gauss- Jordan elimination method; Matrix inversion. Eigen values and Eigen vectors: Jacobi's method for symmetric matrix.

Unit III

Numerical Solution of First Order Differential Equations: First order Taylor Series method; Euler's method; Runge-Kutta methods; Predictor corrector method; Elementary ideas of solutions of partial differential equations, Numerical Solutions of Second Order Differential Equation: Initial and boundary value problems: shooting methods

UNIT IV

Computer basics and operating system: Elementary information about digital computer principles; basic ideas of operating system, DOS and its use (using various commands of DOS); Compilers; interpreters; Directory structure; File operators.
Introduction to FORTRAN 77:Data types: Integer and Floating point arithmetic; Fortran variables; Real and Integer variables; Input and Output statements; Formats; Expressions; Built in functions; Executable and non-executable statements; Control statements; Go To statement; Arithmetic IF and logical IF statements; Flow charts; Truncation errors, Round off errors; Propagation of errors, Block IF statement; Do statement; Character DATA management; Arrays and subscripted variables; Subprograms: Function and SUBROUTINE; Double precision; Complex numbers; Common statement; New features of FORTRAN 90.

Note: The syllabus is divided into four units. Nine questions will be set in all. Question No.1 will be compulsory having four to eight parts covering the whole syllabus. In addition there will be two questions from each unit and the student is to answer one question from each unit. A student has to attempt five questions in all.

Text and Reference Books

[1] Sastry : Introductory methods of Numerical Analysis.
[2] Rajaraman: Numerical Analysis.
[3] Ram Kumar : Programming with FORTRAN 77
[4] Press, Teukolsky, Vellering and Flannery : numerical Recipes in FORTRAN.
[5] Desai: FORTRAN programming and Numerical methods.
[6] Dorn and McCracken : Numerical Methods with FORTRAN IV case studies.
[7] Mathew : Numerical methods for Mathematics, Science and Engineering.
[8] Jain, Iyngar and Jain: Numerical methods for Scientific and Engineering Computation"
[9] Gould and Tobochnik : An Introduction to Computer Simulation methods part I and Part II.
[10] McCalla : Introduction to Numerical methods and Fortran programming.
[11] Verma, Ahluwalia and Sharma : Computation Physics : An Introduction.