Computational Methods in Physics

Programme: M. Sc. (Physics) | Year: 1st year | Semester: 1st semester
Course : Program Core | Credits : 3 | Hours (LTP): 40+0+0

Course Context and Overview (100 words):

Programming skills have become necessary in various fields of study not just Physics. This course teaches the basic concepts of programming techniques with emphasis on solving physics problems.

Prerequisites Courses:

None

Course outcomes(COs):

On completion of this course, the students will have the ability to:	
CO1:	Apply the knowledge of basic concepts of programming to any language of their choice
CO2:	Plot data (2D / 3D) derived from programming / experiments
CO3:	Find roots of equations
CO4:	Solve system of linear equations and
CO5:	Interpolate from given data
CO6:	Numerically perform differentiation and integration
CO7:	Solve Ordinary Differential Equations

Programming language to be taught: C

Course Topics:

Topics	**Lecture Hours**
UNIT I: Introduction to Computers / OS and Basic concepts of Programming	

1. Flow charts, Algorithms	16
2. Integer and floating point arithmetic, Precision, Variable types, Arithmetic statements, Input and output statements,	
3. Control statements, Executable and non-executable statements,	
4. Arrays	
5. Repetitive and logical structures, Subroutines and functions, Operation with files;	
UNIT II: Plotting softwares	2
1. Gnuplot, Grace, Origin **Examples:** a) Application of this in M. Sc. Laboratory Experiments b) Wave function in Quantum Tunnelling c) Radioactive Decay	
UNIT III: Root finding methods	3
1. Graphical Method	
2. Bracket Methods	
3. Open End Methods	
Examples: a) Finding roots of non-linear algebraic equations in Physics	
UNIT IV: System of Linear Equations	5
1. Gauss elimination Method with and without pivoting.	
2. LU Decomposition	
3. Gauss Seidel	
Examples: a) Coupled Harmonic Oscillator b) Heated rod problem	
UNIT V: Interpolation	4
1. Linear Interpolation	
2. Newton's interpolation technique	
3. Lagrange interpolation	
4. Pitfalls in interpolation	
5. Spline interpolation technique	
Examples: a) Application of this technique in M. Sc. Laboratory Experiments	
UNIT VI: Differentiation & Integration	3
1. Difference formulas for 1st order and 2nd order differentiation	
2. Trapezoidal rule	

3. Simpson's rule	
UNIT VII: Ordinary Differential Equations	7
1. Initial value problems	
a) Euler method / Heun's Method / Runge-Kutta method of order four	
2. Boundary Value problem	
a) Shooting method	
b) Finite difference method	
Examples: a) Newton's Law. b) Electrodynamics Problems. c) One dimensional time-independent Schrodinger's Equation	

Textbook references:

Text Book:

1. E. Balagurusamy, *Programming in ANSI C*, McGraw Hill Education India Private Limited.
2. Y. Kanetkar, *Let us C*, BPB Publications, New Delhi 2016.
3. N. Giordano and H. Nakanishi, *Computational Physics*, Pearson/Prentice Hall, 2006.
4. P. DeVries and J. Hasbun, *A First Course in Computational Physics*, New Delhi: Jones & Bartlett Learning, 2011.

Reference books:

1. B. Gottfried, Schaum's Outlines: *Programming in C*, Tata McGraw Hill Education Private Limited, New Delhi, 2011.
2. B. W. Kernighan, D. Ritchie, *The C Programming Language*, Pearson Education Singapore, 2015.
3. J. E. Hasbun, *Classical Mechanics with MATLAB Applications*, Jones & Bartlett Learning, New Delhi, 2012
4. S. C. Chapra, *Applied Numerical Methods with MATLAB for Engineers and Scientists*, Tata McGraw Hill Education Private Limited, New Delhi, 2012.

Additional Resources (NPTEL, MIT Video Lectures, Web resources etc.):