

PHY5204 Computational Physics

Course Code	PHY5204	Semester	II
Course Title	<i>Computational Physics</i>		
Credits	4	Type	Core

Course Outcome

- (1) To train students in using modern mathematical techniques in performing numerical computation.
- (2) To train students in handling modern UNIX based systems
- (3) To teach basic simulation techniques used in physics
- (4) To impart skills in using these techniques in practice

Course Structure

Contents: Numerical methods for solving nonlinear equations, interpolation, system of equations, differentiation, integration and solution of differential equations. Treatment of boundary value problem. Fourier transformation and FFT. Method of least square.

Elements of Unix operating system, Unix tools for science: vi editor, GNUPlot, Latex for typesetting, GCC compilers. Concepts of object oriented programming. Introduction to parallel processing and high performance computing. Detailed study of a high level language like Fortran, C/C++, Matlab/Octave.

Random number generation and Monte Carlo integration. Random walk and percolation models. Numerical solution of Schrodinger equation for one dimensional potentials using finite difference methods. Treatment of hydrogen atom. Periodic potentials and band structure (one dimension). Numerical method of solving equations of motion. Introduction to molecular dynamics and Monte Carlo simulation. Simulation of chaotic systems.

Laboratory work: Practical implementation of numerical methods and simulations in computational lab sessions using any programming language

Suggested Books

1. Tao Pang, Computational Physics, Cambridge
2. D.P.Landau, Survey of Computational Physics, Academic Press
3. Paul DeVries and J. Hasbun, Introduction to Computational Physics,
4. Philipp Scherer, Computational Physics, Springer (2010)
5. N.J.Giordano, Computational Physics, Prentice Hall (1997)