BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE-Pilani,
Hyderabad Campus
FIRST SEMESTER 2022-2023

Course Handout (Part II) Date: 29-8-2022

Course No.: PHY F313
Course Title: Computational Physics
Instructor-in-charge: P.K.Thiruvikraman

Course Description: The use of computers for computation and simulation has become an integral part of physics. This course introduces the basic computational methods that are used to solve problems in Physics. Some of the topics, which will be covered are numerical methods for finding roots (with special emphasis on transcendental equations), solution of differential equations, integration (including Monte Carlo techniques for evaluating integrals). Applications of these techniques will also be discussed in class.

Scope and objective of the course: The objective of the course is to introduce basic techniques for solving Physical problems by using computational methods. Most of the real-world problems are not solvable analytically. An advantage of computational physics is that one can start with an idealized (simplified) version of a real problem for which an analytical solution exists. Once a program has been written that can handle the idealized case, we can add more complex real-world factors. Illustrative examples will be taken from various areas of Physics like Classical Mechanics, Condensed Matter Physics, Electricity and Magnetism, Quantum Mechanics, Statistical Physics etc. Some of the modern topics like Chaos, Percolation and random walk, will also be covered in the course.

Text Book:

First course in Computational Physics by Paul DeVries, Javier E. Hasbun, Jones and Bartlett Publishers, Indian edition, 2011

Reference Book:

1. Numerical Recipes in C, 2nd Edition, W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, Cambridge University Press, 1992.
2. An Introduction to computer simulation methods, 2nd Edition, Harvey Gould and Tobochnik, Addison Wesley,1996.
3. Applied Numerical Analysis, 7th Edition, Gerald and Wheatley, 2003
4. Numerical Methods for Engineers, 6th Edition, Chapra & Canale, McGraw-Hill, 2012
5. Computational methods using MATLAB, P.K.Thiruvikraman, IoP Science, 2022

Course Plan

Lecture No.	*Learning outcomes*	*Topics to be covered*	*Chapter in the Text Book*
1.		Introduction	-
2-6	Finding the Roots of a function by numerical methods	Iteration method, bisection, Newton Raphson method, method of false position, secant method.	2.1- 2.10
7-8	Application of root finding techniques	Finite square well potential	2.11-2.12
9-11	Techniques for Interpolation and approximation	Lagrange interpolation, error in interpolation	3.1, 3.4-3.7
12-14	Matrix methods for solving simultaneous equations and use	Gaussian Elimination, LU decomposition, Least Squares curve fitting	3.10, 3.11-3.14

	them for curve fitting		
15-17	Numerical differentiation and Integration	Trapezoidal rule, Simpson's rules, Gaussian Quadrature and application, Romberg integration	3.8-3.9, 4.1-4.6, 4.8, 4.10-4.13
18-22	Numerical Integration	Random Number generators, Metropolis Algorithm, Monte Carlo Integration and its application	12.6 (R2) & class notes, 11.8 (R2), Chap 4 (TB) & Chap 11 (R2)
23-28	Solve Ordinary Differential Equations	Euler Methods, higher order Runge-Kutta Methods and application, Finite difference method, finite element method	5.1-5.6, 5.16-5.25 (TB)
29-32	Solve Partial Differential Equations	Solution of boundary value problems by finite difference methods and application	Chap 7 (TB) Chap 10.2-10.4 (R2)
33-37	Monte Carlo Simulations	Random walk, Ising model	Chap 4 (TB); Chap 5 (TB), Chap 17 (R2)
38-42	Solution of Non-linear differential equations	Chaos	Chap 6 (TB)

Evaluation scheme:

Component	Duration	Weightage(%)	Date & Time	Nature of Component
Mid-semester test	90 min	30 %	03/11 11.00 - 12.30PM	Open Book
Assignment		15 %		Open Book
Tests (best 1 out of 2)	50 min	15%		Closed book
Compre. Exam	3 hrs	40%	24/12 AN	Closed Book

Chamber Consultation hour: Tuesday 5 PM to 6 PM.

Notices for this course will be displayed on the Course Management System (CMS) website only.

Academic Honesty and Integrity Policy: Academic honesty and integrity are to be maintained by all the students throughout the semester and no type of academic dishonesty is acceptable.

Instructor-in-charge,
PHY F313