COMPUTATIONAL PHYSICS (PH 3304)

AUTUMN SEMESTER (2020-21)

DEPARTMENT OF PHYSICS

NATIONAL INSTITUTE OF TECHNOLOGY, JAMSHEDPUR

Contact Hours: 3-0-1(L-P-T)

No. of Credits:4

Course Instructor: Dr. Neha Agnihotri

Evaluation details:

Total evaluation marks: 100

OBJECTIVE

This course aims to introduce the fundamentals of computational physics and programming.

COURSE CONTENT

UNIT I: (21 Lectures)

Solution of Algebraic and Transcedental equations, Solution of simultaneous linear equations, Interpolation.

UNIT II: (19 Lectures)

Numerical Differentiation, Numerical Integration, Numerical solution of ordinary differential equations, Simulation Techniques, Variational methods and optimization techniques, Applications of computer simulations in physics

READINGS

1. ***Computational Methods in Physics and Engineering: Wong***
2. ***Computer Oriented Numerical Methods: Rajaraman***
3. ***A Guide to Monte Carlo Simulations in Statistical Physics : Landau and Binder***
4. ***Understanding Molecular Simulation (Academic Press): D. Frenkel and B. Smit***

OUTCOME OF THE COURSE

It is expected that students will learn fundamentals of computational physics and programmingwhichwill help them in analyzing the experimental data in further studies. This course will also provide background for the students who wants to carry out research in theoretical physics.

LECTURE-WISE COURSE PLAN FOR PH-3304

S. No.	Topic	No. of Lectures
1.	Errors in Numerical Calculations	02
2.	Solution of Algebraic and Transcedental equations: ***Bisection Method***	01
3.	***Secant Method***	01
4.	***Regula- Falsi Method***	01
5.	***Newton- Raphson Method***	01
6.	***Iteration Method***	01
7.	***Tutorial-1***	02
8.	Solution of simultaneous linear equations***: Gauss Elimination Method***	01
9.	***Gauss-Jordan Method***	01
10.	***LU decomposition Method***	01
11.	***Matrix Inversion Method***	01
12.	***Tutorial-2***	02
13.	Interpolation: ***Newton-Gregory Formula***	02
14.	***Lagrange's Interpolation Formula***	02
15.	***Tutorial-3***	02
16.	Numerical Differentiation	02
17.	Numerical Integration: ***Trapezoidal Rule***	01
18.	***Simpson's 1/3 Rule, Simpson's 3/8 Rule***	02
19.	***Tutorial -4***	02
20.	Solution of ordinary Differential Equations: **Euler's Method**	01
21.	**Runge-Kutta Method**	02
22.	***Tutorial-5***	01
23.	Simulation Techniques: ***Random number generation***	01
24.	***Monte-Carlo Methods***	01
25.	***The Metropolis Algorithm***	01
26.	***Variational Methods, Optimization Techniques***	01
27.	Applications of Computer Simulations in Physics	03
28.	***Tutorial-6***	01