

First-course Handout – PHY 617: Computational Physics – Sem: 2026-27-II

Department of Physics, IIT Kanpur

Instructors: Koushik Pal (koushik@iitk.ac.in); Office: Old SAC (Block C) Room # 106.

Schedule and Location:

Lectures: Tue, Wed, 12:00 – 13:15, (**Venue: TBD**)

Tutorial: Thu, 14:00 – 17:00, (**Venue: TBD**)

Objectives: The objective of this course is to introduce details of numerical computation used in many fields of physics. Students will learn techniques to solve physics-based problem using numerical computation.

Tentative course outline:

- Introduction to computers, Python basics, and visualization.
- Interpolation - Lagrange, Splines.
- Numerical Integration- Newton-Cotes, Gaussian quadrature, Monte Carlo, Numerical differentiation.
- Ordinary differential equation solvers – stability accuracy issues, explicit vs implicit Schemes, predictor-corrector methods (Euler, Runge-Kutta), multistep methods (Adam-Bashforth), Stiff Equations, Leapfrog and Verlet methods.
- Partial differential equation – spectral method, finite difference method to solve parabolic equations – diffusion equation, Schrodinger equation, stiff equations.
- Laplace and Poisson's equations, nonlinear equations – iterative procedure, Newton's method, Secant method.
- Linear Algebra – Matrix eigenvalue problems
- Problems from classical, statistical, and quantum mechanics.

Recommended Books:

- Computational Physics with Python, 2nd Ed., Mark Newmann.
- Computational Problems for Physics: With Guided Solutions Using Python, Rubin H. Landau and M. J. Paez, CRC Press (2018).
- Effective Computation in Physics: Field Guide to Research with Python (O'Reilly Media).
- Python for Computational Science and Engineering by Hans Fangohr.

Evaluation: Mid-semester examination – 30 %, End-semester examination – 30 %, Quiz – 20 %, Assignments - 20%.

Course Policy:

- Attendance is mandatory for this course.
- There will be no make up for quizzes and mid-semester examination.
- Make up for the end-semester examinations will be conducted only if permitted by the DOAA.
- The DOAA [guidelines](#) regarding the use of unfair means will be strictly followed.