IISER Pune - Course Content

Semester	JAN 2026
Open to Semester	6,8,12,14,22,32
Course Code	PH3264
Course title	Computational Physics
Nature of Course	LB - Lab
Credit	4
Coordinator and participating faculty (if any)	Dr. Prasenjit Ghosh Dr. Apratim Chatterji
Pre-requisites	Quantum Mech-1, Statistical Physics-1
Objectives	This advanced course aims to give the students competence in the methods and techniques of calculations using computers. The student will get explore to 7 different computational algorithms/calculations in 6 different modules. At the end of the course the student is expected to have a hands on experience in modeling, algorithm development, implementation and calculation of physical quantities of relevance in interacting many body problems in physics. Both quantum and classical computational tools will be introduced. The hands-on-lab component is 4 to 5 hours a week during contact hours, which will be used in problem solving. The students student will come to class after going through recorded lectures. The expectation is that in future the student will be able to learn on his/her own any computational method that will be relevant the future problem solving (in research or otherwise) and extract reliable trustworthy results. The focus is on the methodologies to implement algorithms and designing multiple levels of checks and cross checks, which the student will develop by implementing the algorithm in the 6 modules.
Course content	Module 0: 1 week : Learning Fortran or C programming Language by implementing the statistical physics of random walks Module 1: 1 week : Random Number generation and testing, Generation of random numbers with given distribution 1 week : Numerical Integration: (a) Deterministic: Trapezoidal method & (b) Multi-dimensional Integration using stochastic methods.

	Module 2 : 2.5 Weeks : Lattice Monte Carlo simulations using Ising model to understand phase transitions: Metropolis algorithm, understanding kinetic barriers, finite size effects, role of thermal fluctuations* calculating thermodynamic averages, Principle of detailed balance, Binders cumulant. Module 3: 1.5 weeks: Solving differential equations, Linear, non-linear and coupled differential equations, Module 4: 1 week Partial differenential equation. Module 5 : 1 week: Solving differential equations Schrodinger eqn. in Quantum Mechanics with Numerov's algorithm Module 6: 1 week : variational principle. Module 7: 2.5 Weeks : Classical Molecular Dynamics simulations using Lennard-Jones' potential, : Classical Molecular Dynamics simulations using Lennard-Jones' potential
Evaluation / Assessment	Continuous evaluation 70%: 10 % for each module. Lectures on each of the topics will complement with hands on sessions where the students will be given assignments which involve developing computer simulation codes as well using standard codes which are available to perform simulations The students will be graded on this performance.) End semester Viva Voce : 30%
Suggested readings	1. Computer Programing in F90 & 95, V. Rajaraman, PHI learning pvt. Ltd 2. Numerical Recipes in F90 Cambridge Publishers 3. Computational Physics by Jos Thijssen (Cambridge Univ Press, 1997) 4. A first course in Computational Physics, P. L. DeVries, John Wiley and Sons. Inc. 5. Understanding Molecular Simulation, Publisher: Academic Press Author: Daan Frenkel and Berend Smit. 6. Monte Carlo Methods in Statistical Physics

	Author- M.E. Newman and G.T Barkema. Publisher : Clarendon Press Oxford. 7. Computer Simulation of Liquids by M. P. Allen and D. J. Tildesley Publisher: Oxford Science Publications.
When Next	January 2027
Date Uploaded	2025-10-29 11:59:12