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| Semester | JAN 2022 |
| Open to semester | 6,8,12,14,22 |
| Course code | **PH3264/PH6234** |
| Course title | **Computational Physics** |
| Credits | 4 /4 |
| Course Coordinator & participating faculty (if any) | Apratim Chatterji |
| Nature of Course | Lectures and Lab |
| Pre-requisites | Stat Mech -1 and Q Mech-1 |
| Objectives (goals, type of students for whom useful, outcome etc) | This advanced course aims to give the students competence in the methods and techniques of calculations using computers. The student will get explore 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.<br><br>The hands-on-lab component is 4 to 5 hours a week. The contact hours, which will be used in problem solving on the computer and clearing doubts. The students student will come to class after going through recorded lectures.<br><br>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 contents (details of topics /sections with no. of lectures for each) | Module 0: 1 week : Rapid overview of Fortran programming Language.<br><br>Module 1: 1 week : Random Number generation and testing, Generation of random numbers with given distribution<br><br>1 week : Numerical Integration: (a) Deterministic: Trapezoidal |

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| | method & (b) Multi-dimensional Integration<br>using stochastic methods.<br><br>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.<br><br>Module 3: 1.5 weeks: Solving differential equations, Linear, non-linear and coupled differential equations,<br><br>Module 4: 1 week Partial differenential equation.<br><br>Module 5 : 1 week: Solving differential equations Schrodinger eqn. in Quantum Mechanics with Numerov's algorithm<br><br>Module 5: 1 week : Quantum problems with variational principle.<br><br>Module 6: 2.5 Weeks : Classical Molecular Dynamics simulations using Lennard-Jones' potential, : Classical Molecular Dynamics simulations using Lennard-Jones' potential |
| Evaluation /assessment | End-Sem Examination-40%<br>Mid-Sem Examination-0%<br>Others-Continuous evaluation: 60%,<br>10% for each module, very much like a lab course.% |
| Suggested readings (with full list of authors, publisher, year, edn etc.) | 1. Computer Programing in F90 & 95, V. Rajaraman, PHI learning pvt. Ltd<br>2. Numerical Recipes in F90 Cambridge Publishers<br>3. Computational Physics by Jos Thijssen (Cambridge<br>Univ Press, 1997)<br>4. A first course in Computational Physics, P. L. DeVries, John Wiley and Sons. Inc.<br>5. Understanding Molecular Simulation,<br>Publisher: Academic Press<br>Author: Daan Frenkel and Berend Smit. |