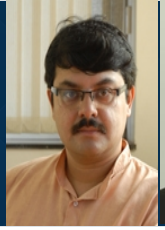


COMPUTATIONAL PHYSICS

PROF.APRATIM CHATTERJI
Department of Physics
IISER PUNE

PROF.PRASENJIT GHOSH
Department of Physics
IISER PUNE

PRE-REQUISITES : Basic Statistical Physics and quantum mechanics.

INTENDED AUDIENCE : Masters students in physics, engineering physics students and scientists interested in quantum and/OR molecular modelling.

INDUSTRIES APPLICABLE TO : Shell, Unilever,TCS

COURSE OUTLINE :

This course aims to give the students competence in the methods and techniques of calculations using computers. 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.

ABOUT INSTRUCTOR :

Prof. Apratim Chatterji has 20 years of research experience in molecular modeling of classical statistical mechanics problems and is active in soft matter research using computational techniques. He joined IISER- Pune in 2009.

Prof. Prasenjit Ghosh is interested in understanding microscopic properties of materials using first principles methods quantum mechanics and classical mechanics based computational methods. He joined IISER Pune in 2010 and has 16 years of research experience in this field. Both the instructors have taught this course in IISER-Pune for 5 semesters with the same course content as given above. At IISER Pune the course is offered to 4 th year BS-MS student, Integrated PhD student and PhD students every year.

COURSE PLAN :

Week 1: Rapid overview of Fortran programming Language

Week 2: Random Number generation and testing, Generation of random numbers with given distribution

Week 3: Numerical Integration: (a) Deterministic: Trapezoidal method & (b) Multi-dimensional Integration using stochastic methods.

Week 4: Lattice Monte Carlo simulations using Ising model to understand phase transitions: Metropolis algorithm, understanding kinetic barriers, finite size effects, role of thermal fluctuations

Week 5: Metropolis algorithm, understanding kinetic barriers, finite size effects, role of thermal fluctuations; Principle of detailed balance, calculating thermodynamic averages

Week 6: Determining transition temperature using Binders cumulant

Week 7: Solving differential equations

Week 8: Linear, non-linear and coupled differential equations

Week 9: Solving differential equations Schrodinger eqn. in Quantum Mechanics with Numerov's algorithm and variational principle.

Week 10: Classical Molecular Dynamics simulations using Lennard-Jones' potential

Week 11: Classical Molecular Dynamics simulations using Lennard-Jones' potential

Week 12: Classical Molecular Dynamics simulations using Lennard-Jones' potential