COMPUTATIONAL SIMULATION METHODS IN PHYSICS(PHY627A)

2×75 minutes Lectures per week, 9 credits – no regular laboratory class, but there will be hands-on sessions whenever required.

This course is open to Ph.D., Master students, and advanced UG students. Basic knowledge of programming is required.

Course content:

C/ FORTRAN programming, revisiting controls/arrays/files, errors, numerical analysis, differentiation, integration, solution of differential equations, solution of Schrödinger equation, simulations of planetary motion, oscillatory motion.

Classical molecular dynamics simulation, simulation of simple gas/liquid, density functional theory (briefly), Ab-initio molecular dynamics simulation (Car-Parrinello method) (briefly), Monte Carlo simulation, simulation of Ising model.

Selected readings:

1. An Introduction to Computational Physics by Tao Pang, Cambridge University press (2006).
2. Computational Physics: A practical Introduction to Computational Physics and Scientific Computing by K.N. Anagnostopoulos (2016).
3. Understanding Molecular Simulation by Frenkel and Smit
4. Computer Simulation of Liquids by Allen and Tildesley
5. Electronic Structure: Basic Theory and Practical Methods by Richard M. Martin