

ICTP DIPLOMA PROGRAMME IN CONDENSED MATTER PHYSICS 2013-14 SYLLABUS

NUMERICAL METHODS II- {9 Lectures = 13.5 hours}

E. Fratini, S. Pilati, A.A. Hassanali

Numerical Linear Algebra:

- Flash review on linear algebra, System of Linear Equation, backward/forward substitution, Gauss elimination, Jacobi's method, finding eigenvalues and eigenvectors, LU decomposition, direct-indirect methods, Power method, hands-on tutorial on LAPACK (diagonalization methods)

Molecular dynamics:

- Flash review of classical statistical mechanics, ergodicity, classical dynamics and integrators (differential equations, Verlet algorithm, stability analysis, thermostats), Interaction potentials (Lennard-Jones, electrostatic, bonded/non-bonded interactions), periodic boundary conditions (long and short range forces), minimum image convention, linear response theory, radial distribution functions, sampling problems and umbrella sampling, hands-on tutorial on MD simulations.

Monte Carlo simulations:

- Markov chains, detailed balance condition, Metropolis algorithm, MC simulations of classical liquids, thermalisation and statistical error analysis, MC simulations of the Ising model, phase transitions (first vs. second order), finite-size scaling, critical exponents, critical slowing down, quantum MC methods based on path-integrals, world-line representation, Bose/Fermi statistics in MC, MC simulations of superfluids, sign problem.