ICTP DIPLOMA PROGRAMME IN CONDENSED MATTER PHYSICS 2014-15

NUMERICAL METHODS I- {15 Lectures = 22.5 hours}

E. Coppola, L. Mariotti, S. Pilati, A. Hassanali

SYLLABUS

Linux Operating System, Unix Commands, bash shell.

Fortran 90 programming: basic operations, input/output, flow control, functions/subroutines, array/matrices, strings, dynamic allocation, use of modules, notions of object oriented programming.

Roots of equations: Bisection, Newton, Secant and Regula Falsi methods.

Integration: trapezium and Simpson methods, Newton-Cotes formulas, Gaussian quadrature.

Ordinary Differential Equations: Euler midpoint method, Runge-Kutta method, introduction to molecular dynamics (Verlet algorithm).

Random Numbers: linear congruent generators, statistical analysis of pseudo-random number generators, non-uniform distributions (transformation method, Box-Muller, rejection method).

Crude Monte Carlo integration: statistical error estimations, importance sampling.

Introduction to Monte Carlo simulations: Markov chains, Metropolis algorithm.