Computer Simulation of Condensed Matter (SIMCON)

1. Introduction

- Models and force fields

- Simulation methodologies

- Basics of FORTRAN

PART I: MOLECULAR DYNAMICS

2. Solving the equations of motion numerically

- Equations of motion

- Finite Difference Methods: Euler, Verlet, Leapfrog, Runge-Kutta and predictor-corrector algorithms

3. Simulating a system of N particles

- Energy and forces

- Periodic boundary conditions

- Short-range forces and minimum image method

- Long-range interactions: Ewald and particle mesh Ewald methods, reaction field

- Thermostats and barostats

- Introduction to quantum methods

PART II: MONTE CARLO METHODS

4. Basics of Monte Carlo simulations

- Metropolis algorithm. Detailed balance

- Monte Carlo integration

- Monte Carlo ensembles: canonical and beyond

- Quantum Monte Carlo methods

PART III: APPLICATIONS

5. Hard Condensed Matter:

- Defects in Solids

- Liquid-solid interfaces, nanomaterials and confined fluids

6. Soft Condensed Matter:

- Polymers

- Biomembranes.

References:

1. D.Frenkel, B. Smit, ***Understanding Molecular Simulation*****,** Academic Press, 2002.
2. J.M.Thijssen, ***Computational Physics***, Cambridge, 2007.
3. 3. *H.Gould, J.Tobochnik, W.Christian,* ***An Introduction to Computer Simulation Methods: Application to Physical Systems,*** Addison Wesley, 2007.

Qualifying system based on:

A. Partial exam (20%)

B. Practices with computer (40%)

C. Final exam: presentation of a MD or MC project (40%)

Final mark = 0.2*A + 0.4*B + 0.4*C

A re-evaluation exam will be carried out if necessary.