Master degree's Programme in Physics of Complex Systems

ADVANCED NUMERICAL METHODS (4 ECTS)
(By G. Bussi & C. Micheletti)

COURSE DESCRIPTION: Introduction to numerical methods applied to molecular dynamics simulations. The course covers the theoretical foundations of molecular dynamics and Monte Carlo simulations, starting from fundamental concepts from Newtonian dynamics, statistical mechanics, and variational principles. The course includes practical sessions where students implementing and applying the algorithms.

EXPECTED LEARNING OUTCOMES: Understanding of basic concepts in statistical mechanics. Capability to execute molecular dynamics simulations in different ensembles.

PRE-REQUIREMENTS: Basic knowledge of the Python programming language. Basic concepts in mechanics (equations of motion, Poisson brackets) and calculus.

COURSE TOPICS

1. Basic concepts of Newtonian dynamics and Statistical Mechanics: energy conservation, time reversibility and phase-space incompressibility, Liouville Theorem, Ergodicity. Derivation of equilibrium statistical mechanics from variational principles (definition of entropy, ideal gas, microcanonical, canonical and grandcanonical statistical ensembles, law of mass acrtion) [10h]

2. Integration schemes for molecular dynamics: Verlet, Trotter splitting, Velocity Verlet. Dependence of the results on the time step. [10h]

3. Sampling the canonical ensemble with Monte Carlo: Metropolis-Hastings rule, balance and detailed balance, hybrid Monte Carlo. [10h]

4. Sampling the canonical ensemble with molecular dynamics: velocity rescaling, Berendsen thermostat, Andersen thermostat, Langevin dynamics, stochastic velocity rescaling. Stochastic equations: Itoh rule, Fokker-Planck equation. [10h]

COURSE STRUCTURE: 30h are devoted to theory classes. 10h are devoted to the correction of computational exercises done independently by the student at home.

READING MATERIALS:

- Kerson Huang; Statistical mechanics
- Julia Yeomans; Statistical mechanics of Phase transitions
- Frenkel – Smith; Understanding Molecular Simulation: From Algorithms to Applications
- Tuckerman; Statistical Mechanics: Theory and Molecular Simulation

STUDY MATERIALS:

For topics 2, 3, and 4: recording of the lectures, handouts, Python notebook with solutions of the exercises

ASSESSMENT AND GRADING CRITERIA: Oral exam.