June 2021

**Lecture «Statistical Physics and Computer Simulation»**

## List of important topics

**Introduction, biological systems and statistics**

- Types of biopolymers
- Basic concepts of statistics
- Random walks and Monte Carlo sampling

**Quantum mechanics and classical mechanics**

- Classical mechanics (Newton, Lagrange, Hamiltonian; with equations)
- Applying constraints (Lagrange multipliers)
- Quantum mechanics (wave-function, operator, correspondence)
- Time (in)dependent Schrödinger formulations (with equations)
- Standard solutions (particle in the box, harmonic oscillator)

**Phenomenological thermodynamics**

- Definitions (system, process, exchanges, …)
- Exchanges (work, heat, matter vs. pressure, temperature, chemical potential; volume work with equation)
- Boundary conditions (different types)
- First law, second law, fundamental equation (with definitions and equations)
- Free energy (Helmholtz, Gibbs; with equations)

**Statistical mechanics – part I**

- Statistical mechanical ensembles (microstates, macrostates)
- Microcanonical ensemble (constraints, distribution)
- Canonical distribution (constraints, distribution; with derivation)
- Boltzmann and Gibbs (Shannon) entropies (equations)
- Partition function, ensemble average (equations)
- Connection to thermodynamics (equations)
- Ergodicity

**Molecular dynamics simulations – part I**

- Levels of resolution
- Computing effort (scaling) for QM and classical methods
- Classical atomistic force fields (terms and functional forms, parametrization strategies)
- Concepts of coarse-graining (parametrization strategies, challenges)

**Molecular dynamics simulations – part II**

- Newton's equations of motion (equations)
- Leap-frog algorithm, Euler method (equations)
- Spatial boundary conditions (finite size/surface effects, ideas/challenges with vacuum, extended wall, periodic boundary conditions)
- Temperature replica exchange (concepts, equations)

**Monte Carlo simulations and stochastic dynamics**

- Monte Carlo sampling (concepts, equations)
- Langevin equation of motion (equations)

**Analysis and interpretation of simulations**

- Preprocessing (coordinate gathering, fitting)
- Statistical analysis (distribution, moments, correlations)
- Properties (most important properties; with equations for $R_{gyr}$, RMSD, RMSF, $D$ and $g(r)$)

**Statistical Mechanics – part II**

- Four most important ensembles (constraints, relevance)
- Isothermal-isobaric ensemble (constraints, distribution, partition function, connection to thermodynamics)
- Grand-canonical ensemble (constraints, distribution, partition function, connection to thermodynamics)
- Fluctuations (derivations, scaling with size)

**Statistical Mechanics – part III**

- Ideal monoatomic gas, Sackur-Tetrode (with equations)
- Factorization of the partition function
- Maxwell-Boltzmann distribution, equipartition (with equations)
- Heat-capacity models (ideal gas, harmonic crystal)

**Thermodynamic boundary conditions**

- Instantaneous temperature/pressure definitions (with equations)
- Thermostating/barostating (feedback mechanisms, various algorithms, practical considerations; with equations for constraint and weak-coupling)
- Grand-canonical simulation (concepts)

**Free-energy calculation**

- Free energy in classical statistical mechanics (main equations)
- Temperature and pressure integration (equations)
- Widom's particle insertion method (equations)
- Direct counting (equation)
- Umbrella sampling and reweighting (equations)
- Concept of thermodynamic cycles
- Thermodynamic integration (equations)
- Hamiltonian replica exchange (equations)
- Free energy perturbation (equations)