Program of the course ED Carnot Pasteur 2025 / 2026

[D4] Computational methods for physical chemistry

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Objectives : Presentation of a numerical simulation technique based on statistical thermodynamics that is largely used in physical chemistry: the classical molecular dynamics simulation

A - GENERAL PRESENTATION (12 hours) :

AI- Introduction (6 h) :

- Statistical thermodynamics : statistical ensembles thermodynamic properties (pressure, temperature) structural properties (correlation functions, spectra, crystallography) dynamical properties (transport coefficients), …
- Simulated systems, atomic models, potentials (ex : Lennard Jones), domains of simulation.

AII- Molecular dynamics (6 h) :

- Comparison between molecular dynamics (MD) and Monte-Carlo methods,
- Equations of motion.
- Algorithms for the solution of the equations of motion,
- Structure of molecular dynamics programs,
- Development of MD algorithms.

B - APPLICATION WORK (4 h) :

BI- Coding the dynamics of a simple system: a string

BII- Use LAMMPS to perform a small simulation of a system of argon particles.