

Potts’model: The Pott’s model is a version of the Ising model in which the spin variable can assume several values. $s_i = 0, 1, \dots, q$. In this project the goal is to write a **Monte Carlo** code to simulate the Pott’s model and evaluate typical observables as done for the Ising model during lectures. Furthermore, we will study the percolation probability, i.e. the probability of having a cluster (of sites having the same spin value) of size similar to the size of the system.

Single File Dynamics: Single File dynamics is a typical expression to indicate the behavior of several Brownian (or Langevin) particles when they diffuse on a line or in a tube but they cannot bypass each other. Using **Brownian dynamics** simulation, the goal is to study the subdiffusive behavior of a tracer particle in such a system. Furthermore, we will investigate generalized correlation profiles in the frame of the tracer [1].

Vicksek’model: The Vicsek model is a mathematical model used to describe active matter. One motivation of the study of active matter by physicists is the rich phenomenology associated to this field. The model consists in point-like self-propelled particles that evolve at constant speed and align their velocity with their neighbours’ one in presence of noise. **Molecular dynamics** simulations based on this model show collective motion at high density of particles or low noise on the alignment [2].

Active Brownian particles model: Active Brownian Particles (ABP) are another paradigmatic model to describe active particles. The model displays a rich phenomenology already at the single particle level. This project aims at investigating, through overdamped **Langevin dynamics**, the behavior of an ABP searching for a target in complex energy landscapes with several metastable basins [3].

Confined Hard Spheres: In the past 20 years, confined liquids have been studied extensively in experiments and simulations, showing that even general questions like whether confinement accelerates or hinders the dynamics depend on the nature of the wall-particle potential or the surface roughness. Additionally, it has been found that confinement even with suppressed layering leads to significant changes in the static and dynamical properties of the liquid. The project aims at investigating the behavior of a liquid confined in a slit or a channel and can be performed using **Monte Carlo** simulations of a hard spheres model or **Molecular dynamics** simulations of particles interacting through a WCA potential.

Lennard-Jones mixtures: Among the intermolecular potentials, the Lennard-Jones (LJ) potential has a central role because it is considered as an archetype model for simple yet realistic intermolecular interactions. Systems including particles with different sizes or different interaction strengths yield excellent glass-forming ability [4]. The goal of the project is to use **NVE or NVT simulations** to study the static and dynamical properties of liquid modeled as a mixture of two different kinds of particles.

Stretching Response of a polymer: Nowadays is experimentally possible to study how biomolecules as proteins or DNA behave when subject to an external pulling force. From a theoretical perspective, such biopolymers may be modeled as chains of particles with excluded volume interaction and some potential which takes into account the chain connectivity. The project aims at investigating the force-extension response of polymers of different lengths by means of **Brownian dynamics** simulations.

References:

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