

# MONTE CARLO AND MOLECULAR DYNAMICS SIMULATION

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## ABSTRACT

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## 1 INTRODUCTION

Many body problems often cannot be resolved analytically because of their huge amount of accessible states, for an instance. In order to solve such a problem with computational assistance, a variety of methods have been developed and all of them have their very own applications and limits. One of the first models is the Monte Carlo simulation with the Metropolis Criterion. Its nature is pure stochastic - the time progression evolves randomly and is not given a set of initial conditions. However, the Molecular Dynamics approach is used for the same initial System - with equal coordinate initialisation and boundary conditions - by solving Newton's equations of motions to all atoms simultaneously. This implies that this kind of simulations are deterministic and can be used to look into a system's time evolution.

The main goal of this work is an implementation of both methods in C++ for a set of noninteracting particles in a finite box with periodic boundary conditions and Lennard-Jones Potential. In order to deepen the similarities and differences in computational and physical aspects, a comparison at the very end is sufficient.

## 2 SYSTEM CONSIDERATIONS

For the scope of this assignment, a system with  $N$  particles in a box of volume  $V$  and temperature  $T$  is considered. The closed box is placed in an external heat bath, hence the total energy is not fixed and the probability  $P_i$  for a given State  $|i\rangle$  with Energy  $E_i$  and  $\beta := \frac{1}{kT}$  is given by

$$P = \exp(-\beta E) . \quad (1)$$

## 3 MONTE CARLO SIMULATION

## 4 MOLECULAR DYNAMICS SIMULATION

## 5 CONCLUSION