MONTE CARLO AND MOLECULAR DYNAMICS SIMULATION

WILLIAM JANKE[1] & ANDREAS HALLER[2]

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ABSTRACT

[1] *wjanke@students.uni-mainz.de*
[2] *ahaller@students.uni-mainz.de*

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 simultaniously. 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 suffitient.

2 SYSTEM CONSIDERATIONS

If not explicitly mentioned, the system's settings are as follows:

N particles in a box of volume V and temperature T are 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

$$P_i = \frac{1}{Z} \exp\left(-\beta E_i\right), \text{ and } Z = \sum_k \exp\left(-\beta E_k\right). \tag{1}$$

Such an ensemble is called canonical or NVT.

3 MONTE CARLO SIMULATION

It has been already mentioned, that MC approaches can be used to research many body systems which are not solvable analytically. Numerical methods simplify this task, but they introduce other challenges - in most cases (especially for large scaling sizes), it is not possible to acces every single state. However, for the explanation of the used algorithm, this can be neglected for now.

3.1 Detailed Balance and the Metropolis Algorithm

Consider the particle flow out of state $|i\rangle$

$$j_i^{out} := \sum_j P_i(t) W_{ij}, \tag{2}$$

with jump probability W_{ij} from state $|i\rangle$ to $|j\rangle$. Analogue, the particle flow into state $|i\rangle$

$$j_i^{in} := \sum_j P_j(t) W_{ji}. \tag{3}$$

This yields to the master equation

$$\frac{dP_i}{dt} = \sum_j \left(P_j(t) W_{ji} - P_i(t) W_{ij} \right), \tag{4}$$

which is fulfilled in the equilibrium by the stricter condition of detailed balance

$$P_i W_{ij} = P_j W_{ji}. \tag{5}$$

In other words - the system moves towards equilibrium if detailed balance is enforced. The key of success is to choose W_{ij} such that detailed balance is fulfilled.

4 MOLECULAR DYNAMICS SIMULATION

5 CONCLUSION