MONTE CARLO AND MOLECULAR DYNAMICS SIMULATION

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ABSTRACT

Twelve years before the start of the series, the Nine-Tailed Demon Fox attacked Konohagakure destroying much of the village and taking many lives. The leader of the village, the Fourth Hokage sacrificed his life to seal the Nine-Tails into a newborn, Naruto Uzumaki. Orphaned by the attack, Naruto was shunned by the villagers, who out of fear and anger, viewed him as the Nine-Tails itself. Though the Third Hokage outlawed speaking about anything related to the Nine-Tails, the children — taking their cues from their parents — inherited the same animosity towards Naruto. In his thirst to be acknowledged, Naruto vowed he would one day become the greatest Hokage the village had ever seen.

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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 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:

Ensemble

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.

Potential and Energy

The particles are interacting via a normed Lennard-Jones Potential

$$V_{ij} = 4\left(\frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}} + \frac{2^7 - 1}{2^{14}}\right), \tag{2}$$

such that $V_{ij} = 0$, if $r_{ij} = 2\sqrt[6]{2}$. The total energy E_n of the system in a state $|n\rangle$ is given by the expression

$$E_n = \sum_i \sum_{j \neq i} V_{ij}. \tag{3}$$

Boundary Conditions

For both implementations, periodic boundary conditions (PBC) will be used. More detailed - the particles at the border of the box can interact with fake

neighbour particles beyond the scope of the border. To understand the principle of this condition, a simple example is sufficient: Consider a one dimensional chain with next-neighbour interacting particles at fixed lattice points. Each one has exactly two neighbours, except for the two at the border. This incident can be terminated when telling the border particles to interact with one another. This yields a positive effect on the system's scale parameters - box length L and number of particles N - they are implicitely bigger without the need for significantly more calculation steps.

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 $|i\rangle$

$$j_i^{out} := \sum_j P_i(t) W_{ij}, \tag{4}$$

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

$$j_i^{in} := \sum_j P_j(t) W_{ji}. \tag{5}$$

This yields to the master equation

$$\frac{dP_i(t)}{dt} = \sum_j \left(P_j(t) W_{ji} - P_i(t) W_{ij} \right), \tag{6}$$

which is fulfilled in the equilibrium (left hand side vanishs) by the stricter condition of detailed balance[1]

$$P_i W_{ij} = P_j W_{ji}. \tag{7}$$

In other words - the system moves towards equilibrium if detailed balance is enforced[2]. The key of success is to choose W_{ij} such that detailed balance is fulfilled. This is accomplished with the Metropolis Criterion

$$W_{ij} = \begin{cases} \exp(-\beta \Delta E) & \text{, if} \Delta E = E_j - E_i > 0 \\ 1 & \text{, if } \Delta E \leqslant 0 \end{cases}. \tag{8}$$

The according proof is short accepting $\Delta E > 0$ without qualification

$$\frac{W_{ij}}{W_{ji}} = \frac{\exp(-\beta \Delta E)}{1} = \frac{\exp(-\beta E_j)}{Z} \cdot \frac{Z}{\exp(-\beta E_i)} = \frac{P_j}{P_i}. \tag{9}$$

1 This is a strong, but not necessary condition to prevent the resulting Markov chain to be trapped in a limit cycle [1].

2 But not in the classical, newtonian way of motion, every snapshot of the system towards equilibrium is the result of random initialised trial steps.

Explanatory Note

This criterion does always accept the trial state, if the energy is lowered and exponentially suppresses those, which raise the energy. For the sake of illustration, all simulation steps will be described in detail.

1. Initialise the coordinates of all particles - random or sorted
2. Perform M trial moves ($M \approx ??$), i.e.
   - Select a particle and move it with vector δr
   - Compute the energy difference $\Delta E = E_j - E_i$
3. Generate a uniformly distributet random number x in $[0, 1]$ and accept the trial move, if eighter $\Delta E > 0$ or $x < \exp(-\beta \Delta E)$, discard otherwise.

4 MOLECULAR DYNAMICS SIMULATION

Molecular Dynamics (MD) gained very much popularity in the 1950 and 1970's to simulate real time behaviour of many body systems or complex structures like proteins.

5 CONCLUSION

REFERENCES

[1] MEJ Newman and GT Barkema. *Monte Carlo Methods in Statistical Physics*. Oxford University Press, 1999.