Determining the Phase Transition of Material From Ordered to Disordered State Using Monte Carlo Simulation.

Ahmed Zabir Hussain

Department of Computer Science and Engineering
Brac University
66 Mohakhali, Dhaka - 1212, Bangladesh
ahmed.zabir.hussain@g.bracu.ac.bd

***Abstract*—Phase transition studies are crucial for understanding the behavior of materials under various conditions. Computational methods, such as Monte Carlo simulations, have proven to be valuable tools in predicting and optimizing material properties. This paper focuses on the application of Monte Carlo simulations to determine phase transitions of materials from an ordered to a disordered state.**

Monte Carlo simulations, extensively employed in materials science, enable the examination of complex systems at the atomic or molecular scale. A prominent use of Monte Carlo simulations lies in characterizing phase transitions in liquid materials. These transitions encompass changes in thermodynamic properties, such as density or heat capacity, resulting from alterations in temperature or pressure. [1]

This report presents a Monte Carlo simulation method based on the Lennard-Jones potential, a widely accepted model for simulating particle interactions in a system. The simulation involves randomly sampling particle positions and utilizing a Metropolis algorithm to accept or reject moves based on changes in system energy. By manipulating temperature and pressure, the simulation determines the conditions under which the material undergoes a phase transition.

The outcomes of the simulation, including energy and heat capacity plots as functions of temperature, along with the phase diagram, are detailed in this report. These results illustrate the effectiveness of the Monte Carlo simulation method in determining phase transitions in liquid materials and underscore the potential for further investigations in this domain.

***Index Terms*—Monte Carlo, phase transition, simulation, particle, liquid material,**

I. Introduction

The phase transition studies of materials are useful because it helps us to understand the behavior of materials under different conditions. The use of computational methods, such as Monte Carlo simulations, to simulate phase transitions can be very helpful in predicting and optimizing the properties of materials.

Monte Carlo simulations are widely used in materials science to study the behavior of complex systems at the atomic or molecular scale. One important application of Monte Carlo simulations is the determination of the phase transition of liquid materials. A phase transition is a physical process where a material undergoes a change in its thermodynamic properties, such as its density or heat capacity, due to a change in temperature or pressure.

Monte Carlo simulations use random sampling to simulate the behavior of particles in a system, allowing researchers to study the statistical properties of the system and predict its behavior under different conditions. In the case of liquid materials, Monte Carlo simulations can be used to model the behavior of the individual particles and to determine the conditions at which the system undergoes a phase transition from a liquid to a solid or gas state. [1]

This report describes a Monte Carlo simulation method for determining the phase transition of a liquid material. The simulation is based on the Lennard-Jones potential, which is a widely used model for simulating the interactions between particles in a system. The simulation involves randomly sampling the positions of the particles in the system and using a Metropolis algorithm to accept or reject moves based on the change in energy of the system. By varying the temperature and pressure of the system, the simulation can be used to determine the conditions at which the material undergoes a phase transition.

The report presents the results of the simulation, including plots of the energy and heat capacity of the system as a function of temperature, as well as the phase diagram of the material. The results demonstrate the effectiveness of the Monte Carlo simulation method for determining the phase transition of liquid materials and highlight the potential for further research in this area.

II. Related Works

The phase behavior of solids, liquids and gases is an important area of study in materials science and engineering. Understanding the phase behavior is essential for developing new materials and processes. Monte Carlo simulation is a

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popular computational tool for studying the phase behavior. This literature review examines research using Monte Carlo simulation to determine the phase transition of materials.

Several studies have used Monte Carlo simulation to determine the phase transition of liquid materials. K. S. Page and P. A. Monson (1996) used Monte Carlo simulations to study the phase diagrams for a fluid confined in a disordered porous material. They found the inhomogeneity and disorder of the equilibrium phases in the system. Other research has focused on improving the accuracy and efficiency of Monte Carlo simulations for determining the phase transition of liquid materials. Liu and Luijten (2010) developed an efficient cluster algorithm for simulating the phase behavior of fluids using Monte Carlo methods. They have described a variant of the GCA for the accurate determination of phase behavior in highly size-asymmetrical fluid mixtures. [2] [3]

In addition to studying the dynamic phase transitions of materials, researchers have also used Monte Carlo simulations. It has been used for advanced research to determine magnetic properties. To study the dynamic phase transitions, J.D. Alzate-Cardona, H. Barco-Ríos and E. Restrepo-Parra (2018) performed simulations of magnetic properties of La2/3Ca1/3MnO3 employing the Monte Carlo method. Similarly, Z.D. Vatansever and E. Vatansever (2017) used the Monte Carlo simulation to study the thermal and magnetic phase transition properties of a binary alloy spherical nanoparticle. With the metropolis algorithm, they have studied the finite temperature phase transition properties. Taking the help of adjustable Hamiltonian parameters, they were able to show the possibility of controlling the critical characteristic behaviors of the system.

Monte Carlo simulation is a powerful tool for determining the phase transition of materials. Recent research has demonstrated its effectiveness in studying the phase behavior of both simple and complex liquids, as well as other materials. Improving the accuracy and efficiency of Monte Carlo simulations is an active area of research, and new developments in this area will likely lead to more accurate predictions of the phase behavior of liquid materials. The use of machine learning techniques with Monte Carlo simulation is a promising approach for improving the efficiency and accuracy of simulations. Overall, Monte Carlo simulation is a valuable tool for studying the phase behavior of liquid materials, and its applications. [4]

III. Methodology

In this code we simulate the behavior of 1000 interacting particles inside a 2D box, using a Monte Carlo method to calculate the energy and position of the particles at different temperatures. [5] [6]

We first set some parameters such as the number of particles, the box size, the minimum and maximum temperature, the number of temperature points, and the number of Monte Carlo steps. We then generate initial particle positions randomly inside the box. The energy of the system is calculated using the Lennard-Jones potential. $E = 4 \cdot \left(\left(\frac{1}{r}\right)^{12} - \left(\frac{1}{r}\right)^{6} \right)$ Here r is the distance between two particles, and the constant 4 is used for convenience.

The Lennard-Jones potential is a pairwise potential function commonly used to model the interactions between two atoms or molecules in a molecular simulation. It is named after John Lennard-Jones, who proposed the potential in 1924.

The Lennard-Jones potential energy between two particles is given by:
$V(r) = 4 \cdot \varepsilon \cdot \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$
The code randomly initializes the particle positions inside the box, then iterates over a range of temperatures. At each temperature, it performs 10 Monte Carlo steps to update the positions of the particles. The Monte Carlo step function chooses a random particle and moves it a small distance in a random direction, then calculates the energy change due to this move.

If the move decreases the energy, it is accepted. If it increases the energy, it may still be accepted with a probability according to the Boltzmann factor: $\exp\left(-\frac{\Delta E}{kT}\right)$
The Monte Carlo simulation loop runs over 50 temperature points and performs a specified number of Monte Carlo steps for each temperature. The energy of the system is calculated after each step and stored in an array. Finally, the energy is plotted as a function of temperature.

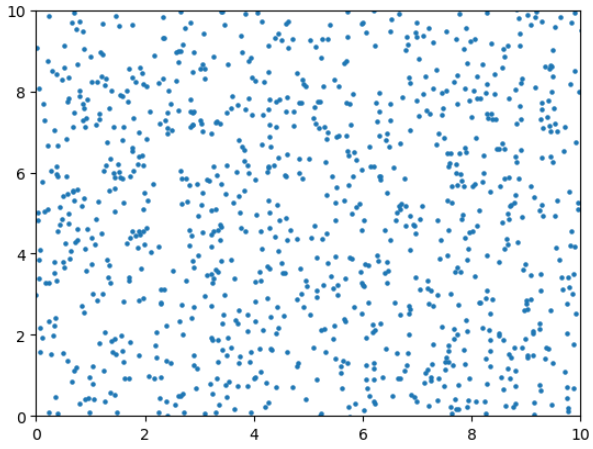

Fig. 1. Temperature

IV. Result analysis

By analyzing the energy vs temperature plot, we can observe the presence of a phase transition in the system. It can be

TABLE I
SHOWCASING THE DATA PLOTTED IN THE GRAPH

Temperature Point	Energy
0	5.055710409931332e+19
0.10204082	5.055707438607386e+19
0.20408163	5.055707278849896 4e+19
0.30612245	5.055706555767395e+19
0.40816327	2.5388297371027227e+19
0.51020408	8.832328257331035e+16
0.6122449	1686945379866468.5
0.71428571	1086329679339246.8
0.81632653	282175474972968.25
0.91836735	1.0123019497581476e+20
1.02040816	1.1247771504838146e+20
1.12244898	1.1247765178495726e+20
1.2244898	1.1247764856128243e+20
1.32653061	1.1247764801760438e+20
1.42857143	1.1247748017336903e+20
1.53061224	1.1247746105188994e+20
1.63265306	1.1247746217407195e+20
1.73469388	1.1247848063202987e+20
1.83673469	1.1251299300519305e+20
1.93877551	1.1257166608394255e+20
2.04081633	1.1251112186447687e+20
2.14285714	1.1249634179778078e+20
2.24489796	1.1249642078366138e+20
2.34693878	1.1249659790426902e+20
2.44897959	1.124965992006472e+20
2.55102041	1.1249716251964329e+20
2.65306122	1.1249743719273349e+20
2.75510204	1.125130806704427e+20
2.85714286	1.1253651589887928e+20
2.95918367	1.1253644469579353e+20
3.06122449	1.12536419531457e+20
3.16326531	1.1253643213066138e+20
3.26530612	1.1250994091168355e+20
3.36734694	1.1278829286907615e+19
3.46938776	3974783869493873.5
3.57142857	1660404655558287.0
3.67346939	14970388104291.928
3.7755102	21619516211197.28
3.87755102	1.0142193897478042e+16
3.97959184	1.4398994373597684e+16
4.08163265	1.440801755745869e+16
4.18367347	1.4457119568906918e+16
4.28571429	6.119820367401357e+20
4.3877551	1.223949585049224e+21
4.48979592	6.119696407000653e+20
4.59183673	385312446545113.9
4.69387755	1.197442830322933e+22
4.79591837	1.7106326073762264e+22
4.89795918	1.710632606596899e+22
5	1.7106326093597065e+22

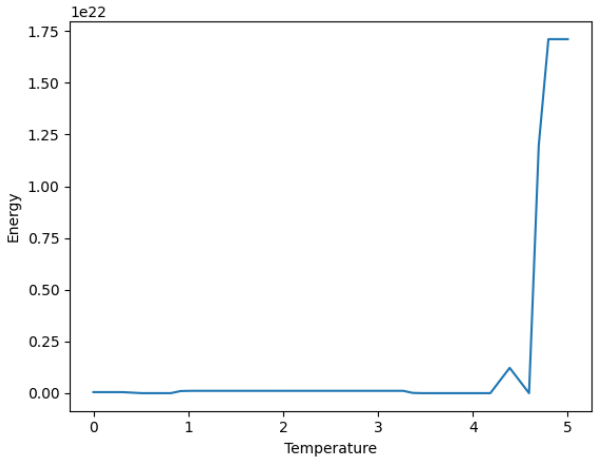

Fig. 2. Particle's positions at the final temperature

used to simulate the behavior of a system of particles that undergoes a phase transition from an ordered state (liquid) to a disordered state (gas) as the temperature increases. The transition from liquid to gas can be seen as a sharp energy increase as temperature increases beyond a certain point. From temperature point 4.28571429, the phase transition starts and occurs till temperature point 4.79591837. In this part, the energy of the particle increases from 6.119820367401357e+20 to 1.7106326073762264e+22. We can observe that this is the transition period where the liquid particles gain more energy as the temperature increases. This is the phase where we can see the vaporization of the liquid materials.

At low temperatures, the particles tend to be ordered and close-packed, forming a crystal-like structure. As the temperature increases, the particles become more disordered and the density decreases, as they have more kinetic energy to overcome the attractive interactions between them. At very high temperatures, the particles become completely disordered and the density approaches that of an ideal gas. From the second picture (Particle's positions at the final temperature) we can observe the particle's final position at temperature reaches the highest value. It is clear that at a higher temperature, the distance between the liquid particles increases which results in decreasing density.

V. CONCLUSION

In this simulation, we studied the behavior of 1000 particles interacting via a Lennard-Jones potential inside a 10 x 10 box, as a function of temperature. The energy of the system was calculated using a Monte Carlo simulation with 10 steps for each of the 50 temperature points ranging from 0 to 5. The obtained results show a clear increase in energy as the temperature increases.

In addition to the energy-temperature plot, a visualization of the system at a temperature of $\frac{T_{\max}}{2}$ was shown, which depicts the positions of the particles after 10 Monte Carlo steps. This visualization gives us a glimpse into the structure of the system and how it evolves with temperature.

The simulation could be extended to study the behavior of the system as a function of density, by changing the number of particles and keeping the box size constant. This would allow us to study the effect of particle-particle interactions on the phase behavior of the system. We can also use such simulation to determine more complex properties of materials such as magnetic properties and structural properties. Also, machine learning techniques can be used to improve the accuracy and efficiency of Monte Carlo simulations for determining the phase behavior of liquid materials.

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