Studying Heat Flow and Magnetization profile of the Ising model using Demon algorithm

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In this paper, we study the heat flow in 1-D Ising lattice using the Demon algorithm. We assign one demon at each site of the lattice to study the local fluctuations in temperature and to determine the temperature gradient, heat flux and the thermal conductivity of the lattice. Lastly, we use the same idea to compute the magnetization profile when the end spins of the 1-D and 2-D Ising lattice were fixed.

1 Introduction

The Monte Carlo simulations has led to important insights into fundamental processes of various systems undergoing complex behaviour. They help us study various dynamical system such as the liquid vapour phase transition or the phase transition in magnetic systems. However, in the usual Monte Carlo algorithm, we keep the temperature fixed by the prescribed interaction of the dynamical system with a heat bath [**harris1988thermal**]. One such example would be the Creutz algorithm where a single demon is assigned to exchange energy with all the spins of a given Ising lattice and the temperature of the system at any point is determined by the energy that the demon has at that instant. Thus, the demon energy governs the temperature of the whole lattice. However, in this paper, we have assigned one demon at each site of the Ising lattice, such that the demon for any i^{th} site only updates the energy of that site. In this way, demons at different sites had different energies, which eventually gave us the local temperature of each site. This allowed us to study the local temperature fluctuation in a non-equilibrium steady state. We have studied the heat flow in the lattice and thus we have drawn its temperature profile by plotting the temperature as a function of site number. Moreover, we have determined the value of the Heat flux Q, which is the energy flow per unit length per unit time, and further we have used Q to determine the thermal conductivity of the given Ising lattice. In the later part of the paper, we have plotted the magnetization profile for the 1-D and 2-D Ising lattices with various boundary conditions.

1.1 Interactions between magnetic spins

In the course of this paper, we will be looking at the interactions between magnetic spins. A chain of these magnetic spins constitutes an Ising lattice. In a simple one-dimensional Ising lattice of N sites, each site i has a spin s_i associated to it, where $s_i = \pm 1$. The Hamiltonian for this Ising lattice is given by,

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i \tag{1}$$

where h is an externally applied magnetic field. The first terms signifies that we are only looking at nearest neighbour interactions and thus it gives us the interaction energy of the neighbouring spins. The *Exchange constant* J is the measure of the interaction between the nearest neighbouring spins. However, the second term represents the interaction between the magnetic moments of the spins and the external magnetic field.

Now, let's assume just two neighbouring spins in absence of any external magnetic field. If we consider both the spins to be parallel to each other, the energy of such a configuration would be $-J$. However, if we assume both the spins to be anti-parallel to each other, we will see that the energy becomes $+J$. Thus, by looking at the energy of these two configurations, we

can say that the parallel alignment is the most stable state and the anti-parallel state is the most unstable state.

1.2 The Demon Algorithm

The Demon algorithm is a very efficient Monte Carlo procedure that is used to sample members of a microcanonical ensemble with a given energy. In this process, we add an extra degree of freedom, called the *'demon'*, which is used to add and provide energy to the system. If a chosen microscopic state has lower energy than the original state, the demon gets the excess energy. However, if the microscopic state has higher energy than required, the missing energy is provided by the demon. If one demon is used, in thermodynamic equilibrium with a system of N spins, it has $(1/N)^{th}$ of the total energy. Thus, the system approximates a microcanonical ensemble with a single temperature. However, in this paper, we will be using one demon per site, which allow us to monitor *local* temperature fields. In either case, the total energy of the spins plus demons is conserved, but there can be local fluctuations of the energy of the spins over short length and time scales, which give rise to thermal diffusion.

1.3 Ising chain as a conductor of heat

As we have discussed in 1.1, for $h = 0$, the energy profile of a spin at a given site of the Ising lattice mainly depends on the spin configuration of its nearest neighbour spins. Thus, we can modify the energy profile at any site by just modifying its nearest neighbour spin configuration. For a 1-D Ising chain of N spins, by keeping the 0 and 1 spin in the highest energy state and the $N-2$ and $N-1$ spins in the lowest energy state (Fig-1), we can get an energy difference at the two ends of the Ising lattice. This energy difference will allow the heat to flow from the higher energy end to the lower energy end. Thus, we can study the heat flow by providing energy at one end and extracting it from the other end of the Ising chain.

Figure 1: Ising chain having the leftmost end with high energy configuration acting as a heat bath and the rightmost end with a low energy configuration acting as a sink.

1.4 Determining the Temperature

The temperature T as a function of the energy of the system can be determined in two ways. One way is to determine the probability that the demon has energy E_d because we know that this probability is related to the demon energy as,

$$P(E_d) = \frac{1}{Z} e^{-\frac{E_d}{k_B T}} \tag{2}$$

where Z is known as the partition function. Thus, by plotting the logarithm of the probability as a function of the demon energy, we can easily determine the temperature of the system. Another way to determine the temperature is to calculate the mean demon energy of the system. However, since the possible values of the demon energy is not continuous for an Ising model, the temperature is not simply proportional to the average demon energy. Rather for $h = 0$ and the limit of an infinite system, the temperature is related to the average demon energy as,

$$\frac{k_B T}{J} = \frac{4}{\ln\left(1 + \frac{4J}{\langle E_d \rangle}\right)} \tag{3}$$

2 Computational Description

The code file that is used to carry out these simulations is attached in the Appendix. The boundary conditions that we have used is a slight modification of the Ising lattice. We have fixed the first two spins of one of the ends to stay anti-parallel throughout the simulation. While the last two spins of the other end are kept parallel to each other (see Fig- 1). Now, in one Monte Carlo simulation, we are sending one demon at each site to update the energy of the given site. However, the demons at the two ends satisfy different conditions than the other demons. The demon at spin 0 adds energy to the system by flipping this spin so that stays in the highest energy state, that is, in the opposite

direction of spin 1. The demon at spin $(N-1)$ removes energy from the system by flipping spin $(N-1)$ so that it stays in the lowest energy state, that is, in the same direction as spin $(N-2)$. As a result, energy flows from site 0 to site $(N-1)$ via the demons associated with the intermediate sites. In order that energy not build up at the hot end of the Ising chain, we require that spin 0 can only add energy to the system if spin $(N-1)$ simultaneously removes energy from the system [**gould1996introduction**].

The temperature of any site is determined by using equation-3. To control the temperature gradient through the system, we have updated the end spins with a higher rate than that of the intermediate spins. We are running our simulations for different number of Monte Carlo sweeps of the order of 10^7.

2.1 Defining initial lattice

In our simulation, we first define the initial spin configuration of our lattice for some desired energy in the following steps;

1. Make a 1-D lattice of N spins, all spins pointing upwards.
2. Flip a random spin in the lattice and calculate total energy of the lattice.
3. Repeat step-2 until the total energy becomes equal to the desired energy.
4. Once step-3 is achieved, stop flipping and return the energy and lattice to be used for initial conditions.

2.2 OneMCS function

We follow the following algorithm to write the one mcs function;

1. If it is $\mathbf{timeToAddEnergy}$:
2. Check if $\mathbf{spins[N-1]}$!= $\mathbf{spins[N-2]}$
3. If yes, then flip $\mathbf{spins[N-1]}$ and add $\mathbf{dE}$ to $\mathbf{systemEnergy}$ and subtract from $\mathbf{demonEnergy[N-1]}$.
4. If last spin was flipped, check if $\mathbf{spins[0]} = \mathbf{spins[1]}$.
5. If yes, then flip $\mathbf{spins[0]}$ and add $\mathbf{dE}$ to $\mathbf{systemEnergy}$ and subtract from $\mathbf{demonEnergy[0]}$.
6. Pick a random index $\mathbf{i}$ from $[\mathbf{1}, \mathbf{N-1}]$.
7. Check if $\mathbf{dE} <= \mathbf{demonEnergy[i]}$.
8. If yes, then flip $\mathbf{spins[i]}$ and add $\mathbf{dE}$ to $\mathbf{systemEnergy}$ and subtract from $\mathbf{demonEnergy[i]}$.
9. Repeat from step $6 \rightarrow 8$ for $\mathbf{N}$ times.

2.3 Defining simulate function

1. Define $\mathbf{demonEnergy[mcsweeps, N]}$, $\mathbf{spins[mcsweeps, N]}$ and $\mathbf{systemEnergy[mcsweeps]}$.
2. Set $\mathbf{demonEnergy[0]} = 0$. For $\mathbf{systemEnergy[0]}$ and $\mathbf{spins[0]}$, use $\mathbf{initial\ lattice}$ values. .
3. Run the $\mathbf{oneMCS}$ function for n Monte Carlo Sweeps, where $n \approx 10^7$.
4. Using previous sweep $(\mathbf{mc-1})$ values; $\mathbf{demonEnergy[mc-1]}$, $\mathbf{spins[mc-1]}$ and $\mathbf{systemEnergy[mc-1]}$, calculate values for current $\mathbf{mc}$ sweep.
5. Return total $\mathbf{systemEnergy}$ and the $\mathbf{demonEnergy\ \&\ spins}$ at each site after n Monte Carlo steps.

3 Results

3.1 Heat Flow in 1-D Ising model

For modelling local temperature fluctuations on a 1-D Ising model, we made our calculations for N = 100 and Monte Carlo sweeps to the order of 10^7 to reach a steady state. We saw that the energy difference between the two ends of the Ising chain allows us to study the heat flow through the system. The temperature profile after n MCS ($n \approx 10^7$) is plotted in Fig-2.

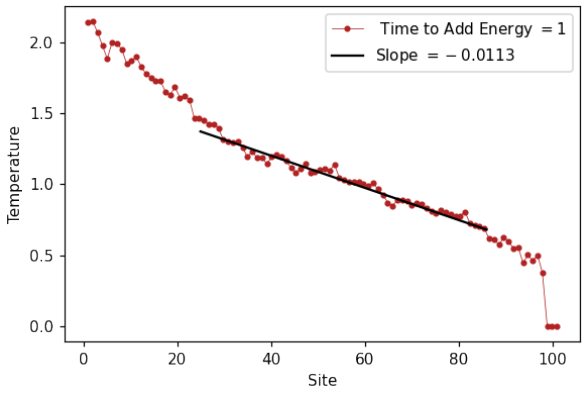

Figure 2: Temperature Profile when the spins on the boundaries of the Ising chain were updated after every Monte Carlo sweep (after average update of N spins). Curve was fitted with a straight line for middle of the lattice (spins 25-85) to avoid edge effects. The slope was obtained to be -0.0113.

From the temperature profile in Fig.2, we can see that site 0 has the maximum temperature, which gradually decreases as we move towards the other end of the chain. The lowest temperature can be seen at the last site, which is consistent with our theoretical assumption. Moreover, the slope of the above plot gives us the temperature gradient $(\frac{\partial T}{\partial x})$. In order to avoid the discrepancy caused due to the edge effects, the temperature gradient was estimated by doing a linear curve fit of the temperature profile in the middle of the lattice only (from site 20-80) [**wang2011thermal**]. Thus the temperature gradient in the given Ising lattice was obtained to be $\frac{\partial T}{\partial x} = -0.108$.

Since, the temperature gradient was not too large, we used the following relation between the heat flux and the temperature gradient to determine the thermal conductivity of the Ising lattice;

$$Q = -\kappa \frac{\partial T}{\partial x}$$

where κ is the thermal conductivity.

Heat flux Q was obtained by determining the energy flow per unit length per unit time. The energy flow is the average amount of energy that demon 0 adds to the system at site 0 and the time is measured in terms of Monte Carlo steps per spin. We monitored the total energy supplied to the system, which for time steps of the order 10^7 was obtained to be $314J$. Since the separation of the two sites was unity and the heat flux came out to be 3.14×10^{-5}. For our calculations, the value of the thermal conductivity then came out to be $\kappa = 0.0028$, when the mean temperature of the Ising chain is 1.605.

3.2 Magnetisation profile for fixed boundary spins in 1-D and 2-D Ising model

For 1-D Ising model

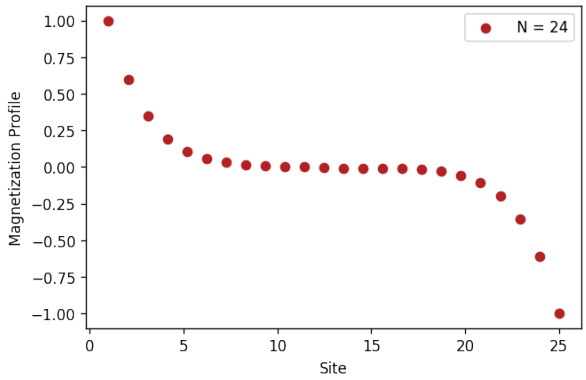

Figure 3: Magnetisation profile obtained for 1-D Ising Model of $N = 24$, when the first and last boundary spins were constrained to be $+1$ and -1 respectively.

The boundary spin 0 was constrained to be $+1$ while the $N - 1$ spin was constrained to be -1. After simulating for over 10^7 Monte Carlo sweeps, the average magnetisation at each site was obtained. Fig. 3 shows the magnetisation profile obtained when calculated for a chain of length $N = 24$. This was done by obtaining the mean value of spin at each site over all Monte Carlo sweeps. For increasing values of N but for the same number of time steps, we obtain the curve to be steeper around the boundaries and flatter for internal spins. Magnetization profiles for higher values of N are attached in the appendix. The temperature profile for an Ising 1-D chain of non-uniform magnetisation was obtained to be uniform [**casartelli2007heat**]. Fig. 4 shows the temperature profile for various values of N, from where we can visually infer that the temperature throughout the chain remains almost same. Thus, we can say that the system is in a thermal equilibrium even when the magnetisation profile is not same.

In the next part, we will observe the effects of the constraint on the end spins for a 2-D case of an Ising lattice.

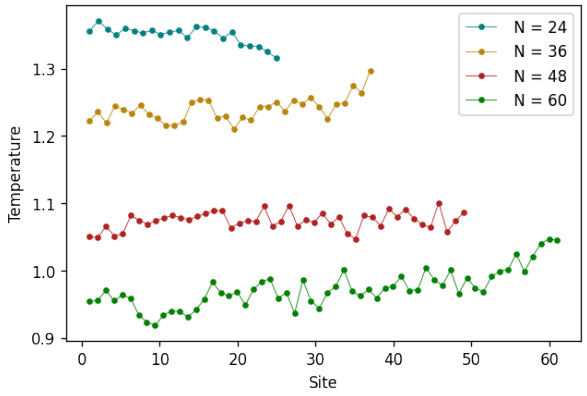

Figure 4: Temperature profile obtained for various lengths of Ising chain, for a system with non-uniform magnetisation. We also observe that the mean temperature at each site reduces as the length of the Ising chain (N) is increased.

For 2-D Ising model

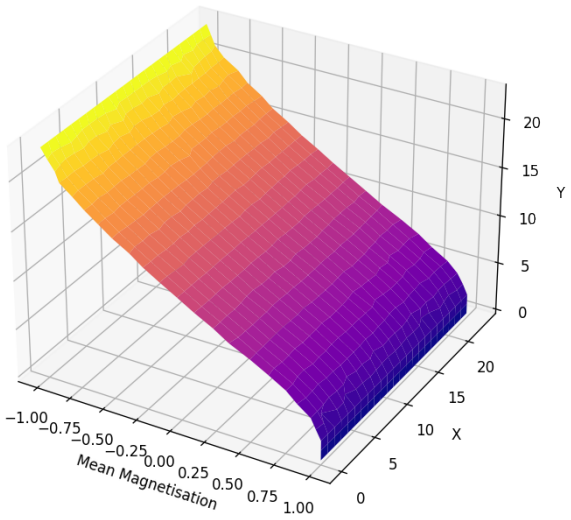

Figure 5: A surface plot for the magnetisation profile obtained for a 2-D Ising model ($L \times L$) of $L = 24$, when the first and last rows of the lattice were constrained to be $+1$ and -1 respectively.

For 2-D case, the constraints on the boundary spins were kept in one direction while keeping the boundary spins in the other direction to be periodic. For a 2-D Ising lattice ($L \times L$), with index i representing the rows and j representing the columns, all spins at $i = 0$ were constrained to be $+1$ and all spins at $i = L - 1$ were constrained to be -1. This gave a cylindrical Ising model with periodic boundary conditions in y-direction while fixed boundaries in x-direction. Fig. 5 shows a surface plot for the magnetisation profile

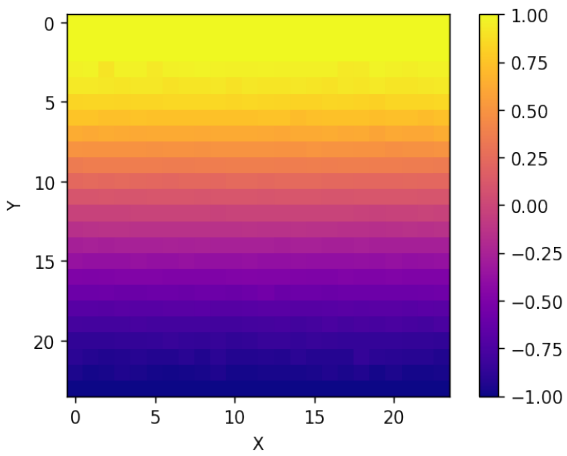

Figure 6: A color plot of the magnetisation profile on a $X - Y$ lattice.

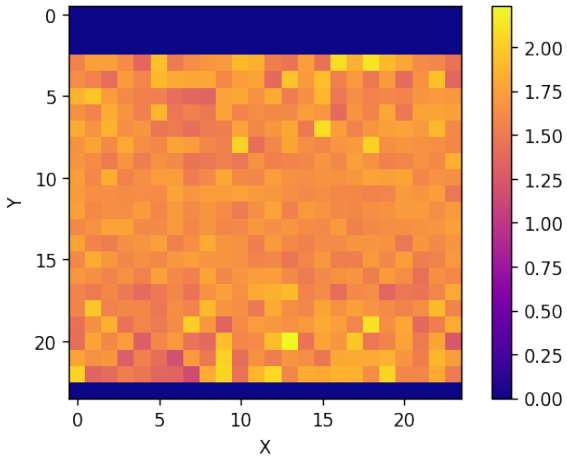

Figure 7: A color plot of the temperature profile on a $X - Y$ lattice.

obtained for 2-D lattice, with mean spin value at each site of a 2-D lattice calculated for all Monte Carlo sweeps. Fig. 6 shows a color plot of the magnetisation profile on a $X - Y$ lattice. From this, we infer that the magnetisation is constant in the X-direction, and is flowing in the Y-direction. Two cross-sectional plots from Y-axis and X-axis of the lattice were also plotted and are attached in the appendix. Fig. 7 shows the mean temperature at each site on the 2-D lattice. Even though the values for the mean temperature at each site ranges from a minimum temperature value of 1.158 to a maximum temperature value of 2.231 (ignoring the temperatures at the boundaries), we can visually infer that there is no temperature gradient in any particular direction. Thus the temperature is overall constant ignoring fluctuations which occurred because the system did not stabilize in the given number of

time steps.

Special boundary conditions for 2-D Ising model

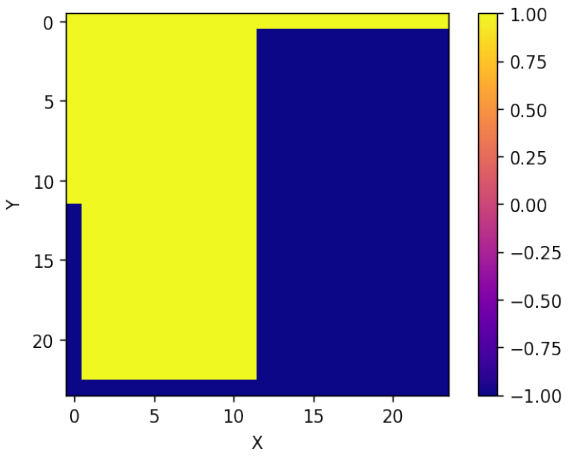

Figure 8: Color plot of the initial spin configuration along with forced boundary conditions but without any update in the internal spins.

The periodic boundary conditions in the y-direction were removed and the spins for $j = 0$ were constrained from $i = 0$ to $(L/2) - 1$ to be $+1$ and $i = L/2$ to $L - 1$ to be -1. The spins at the first and last rows of the lattice were also constrained to be $+1$ and -1 respectively. A color plot of boundary conditions to be enforced at each time step is attached in the appendix. An initial configuration where all the spins on left half of the system (from $j = 0$ to $(L/2) - 1$) are $+1$ and the other spins (from $j = (L/2)$ to $L - 1$) are -1 was chosen for the system. Fig. 8 shows the color plot when the initial configuration was first enforced with the boundary conditions without any update in the internal spin. After simulating the system for 10^4 time steps, the final Fig. 9 shows for various lattice sizes,the final configuration of the spins, after simulating the system for 10^4 time steps and allowing it to reach equilibrium. The magnetization profile for such boundary conditions, obtained for various lattice sizes is also attached in the appendix. From Fig. 9, we observe that when the system was allowed to relax constrained to the boundary conditions, the spins aligned -1 dominates the lattice from lower side of the lattice and a domain wall is formed. The reason for such special separation is because the -1 spins dominates initially on the boundaries of the lattice. Even though the column $j = L - 1$ is not constrained to be -1, the initial configuration supplied forces all spin values of that column, except for $i = 0$, to take the value of -1 (See Fig. 8). Since we do not have the periodic boundary condition in the y-direction, the initial effect of the last column relaxes the system such that it gets dominated by the spin values of -1. From Fig. 9 we also infer that as the lattice size grows, the domain wall becomes smooth and for $L \to \infty$, we expect it to become a straight line connecting mid-point of the column $j = 0$ to the top point of the column $j = L - 1$. As a result we expect the spin values of $+1$ to take one-fourth of the lattice size and the rest dominated by -1 spin values.

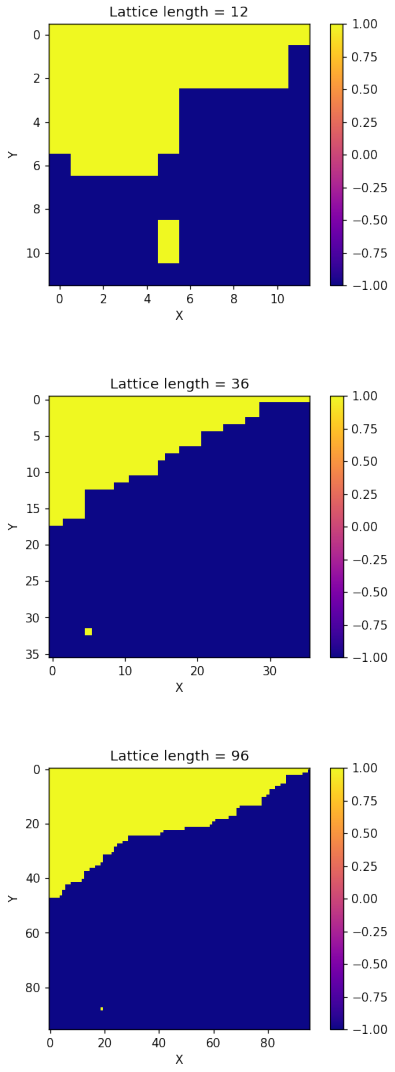

Figure 9: Color plot of the final configuration of the spins once the system has reached equilibrium after simulating over 10^4 time steps, done for lattice of various lengths.

4 Conclusion

In this paper, the results that we got from the study of the heat flow in 1-D Ising lattice signifies the possibility of using Ising lattice to model heat flow in various systems. The value of the thermal conductivity that we got was of the same order of the thermal conductivity of the inert gases like Krypton ($\kappa = 0.0088$), Radon ($\kappa = 0.0033$) etc.
In the later part of the paper, we have used the demon algorithm to obtain the magnetisation profile when the boundary spins of the lattice were constrained. For 1-D case, we obtained that the system was in thermal equilibrium for a non-uniform magnetisation. We also obtained the magnetisation profile for a 2-D cylindrical Ising model and for a special boundary condition case.

5 Discussion

While plotting the temperature profile of the 1-D Ising lattice, increasing the number of Monte Carlo Steps might give us better results of the heat flux and the thermal conductivity of the system. No relation between the thermal conductivity and mean temperature of the Ising chain was established for our system. However, for any general conductor, thermal conductivity is a property of the mean temperature of the conductor. Moreover, one can extend the code to two-dimensions to study the heat flow in a 2-D Ising lattice that can give us much more interesting results. The area of study is active in research on thermal transport and thermal management in nanoscale systems.[**saito1999transport**] The most fundamental thermal device is a thermal diode, which provides a one-way traffic road for heat flow, namely, it allows heat flow in one direction but forbids heat flow in the opposite direction. Our system also tries to simulate one such system which allows heat flow in one particular direction, with a known thermal conductivity. Since, other kinds of algorithms, such as Metropolis algorithm are applicable only to equilibrium state while heat conduction is a typical non-equilibrium phenomenon. Thus, in order to study such non-equilibrium state, the dynamics of the model must be studied, which was done for our paper.