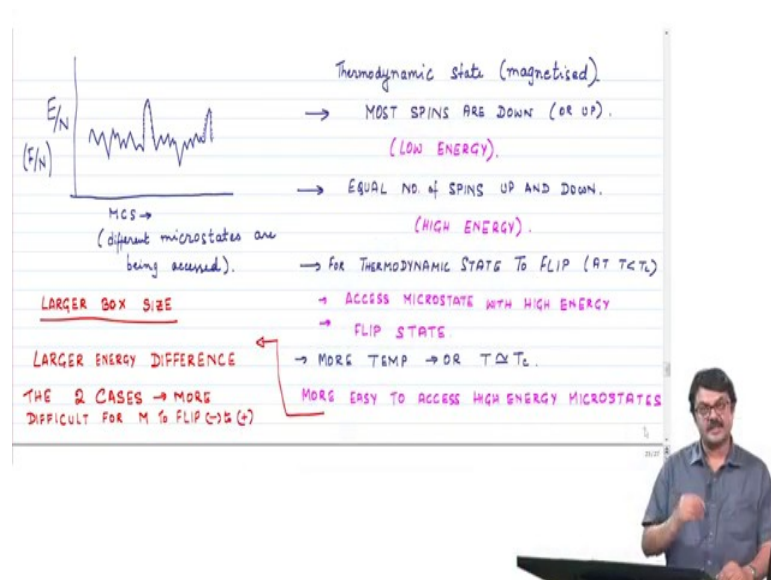


Computational Physics
Dr. Apratim Chatterji
Dr. Prasenjit Ghosh
Department of Physics
Indian Institute of Science Education and Research, Pune

Lecture - 22
Monte Carlo Simulation Analysis Part 02

The question we have to address is that why is it that the magnetic state of the system is going from negative to positive. And again after sometime positive back to negative and this flip keeps on happening; and why as we increase the lattice size the frequency of such flips becomes fewer.

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So, to understand that let us go back to the board. So, here what we have plotted is the Energy Per Spin versus Monte Carlo Steps. So, as different Monte Carlo steps are being accessed basically the system is going from one micro state to the other. Now as it goes from one micro state to the other basically the energy is fluctuating it is going up down as the number of flip, as the number of spins are flipping.; But at a time once in a while the state the system accesses very high energy, relatively high energy as here; and then again it starts fluctuating and it can go down and so on so forth. But once in a while it accesses relatively high energies.

Now, consider a system suppose 20 cross 20 lattice, if the temperature is less than T_c , that is the state is magnetized; the thermodynamic state is magnetized most spins are pointing up or say down does not matter, right. Most of the spins are pointing either down or up, but there are a few which are pointing in the opposite direction. So, they are forming small domains, this is a relatively low energy state. So, basically the average energy of that microstate is low, it is close to minus 2 per spin, right; some higher value than minus 2 per spin.

Now, once in a while this system can access energy from the external heat bath, which we have not directly modeled and it can access high energy microstates. When it goes to high energies and really high energies relatively speaking, then you could have a microstate where you have approximately equal number of spins pointing up and down.

And then when it tries to access back low energy microstates, it is possible that suppose initially before accessing the high energy microstate most of the spins were up; then it goes to a high energy microstate where if there is equal number of spins which are pointing up and down. And while relaxing back to a lower energy microstate it goes to a microstate where most of the spins are pointing down; most of the spins pointing up and most of the spins pointing down I have an equal amount of energy. And basically to go for the magnetic state of the system to flip from up to down or down to up intermediate steps it has to access this high energy microstate. And as you increase suppose the temperature the probability of accessing these high energy microstates becomes higher.

So, if you notice carefully as I took the temperature close to 2.1, 2.15, the frequency of the spin not the spin, but the magnetic state of the system became more frequent. So, they were more frequent from plus to minus, minus to plus and so on so forth; whereas, if you are lower temperatures say at 1.8 or 1.5 the transition temperature being above 2.2. Then you there is a much lower frequency of seeing these flips from one magnetic state to the other from positive to negative.

So, basically increasing temperature increases the frequency of these flips, because higher energy microstates are easily accessible. Of course, above the transition temperature, the average magnetic state of the system is on an average half of the spins are up and half of the spins are down. Here we are talking about the system and the temperature is less than T_c , right.

Moreover if you have a larger box size; while we were plotting the data, we were plotting energy per spin or magnetic state per spin, magnetization per spin. But if you have a larger box size basically the average energy of the system the entire system at T less than T_c is much lower compared to a lower box size, right. Now, when the system has to access the higher energy state, when all spins are up; a half of them are up and half of them are down,; their energy difference between the low energy microstates and the higher energy microstates is much higher, if you have a much larger box size.

So, the amount of energy that the system has to absorb, say from the heat bath the external heat bath is much higher; and hence, the probability of accessing these high energy microstates which have equal number of spins pointing up and down becomes much less frequent. And hence even the flip from the state, from say the positive to the negative state; remember the all these are magnetized states we are talking about T less than T_c , yet we are seeing these flips.

So, if you have a larger lattice size then you have a lower probability of accessing those high energy microstates with equal number of spins pointing up and down. Hence the probability of that the state of the system will flip from positive to negative or negative to positive also becomes lower, right. And that is exactly what we saw in our data when we were analyzing the data.

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HOW DO WE CALCULATE THERMODYNAMIC AVERAGES $\langle M \rangle$?

- $\langle \ln(M) \rangle$ → will lead to finite $\langle M \rangle$ at $T > T_c$.
- APPLY SMALL \vec{B} field at Large box sizes.
 - one broken symmetry is chosen by the system.
 - Take $N \rightarrow \infty$ limit. and calculate $\langle M/N \rangle$.
 - $\vec{B} \rightarrow 0$

FURTHERMORE $\langle M \rangle/N, \langle E \rangle/N, \langle E^2 \rangle, \langle M^2 \rangle, \langle M \rangle, \langle E \rangle$ } C_v, χ

AT EACH T (TEMP).
let system equilibrate for N -equil MCS.

Now that creates a problem. The problem is, if you have a finite size of the lattice, right; how do we calculate thermodynamic averages specially at temperatures which is lower than T_c ? Because if we take a really good thermodynamic average, right and you run it for a really large number of Monte Carlo Steps; then for any finite system on the magnetization specially close to T_c or at relatively higher temperatures lower than T_c ; the system might be magnetized. But the magnetic state of the system can go from positive for a negative, negative to positive.

And if you take an average of the magnetization; what do I mean by average of the magnetization? Calculate the instantaneous magnetization at different Monte Carlo steps and average them over. So, that will give you the average magnetization, so right. So, you are taking an average over the instantaneous magnetization; which we have not done till now. Till now what we have been looking at, the how does the instantaneous magnetization fluctuate with MCS.

But now if your average over the number of Monte Carlos Steps to calculate the so called thermodynamic magnetization. Now, in a finite lattice half of this time the magnetization of the state, the instantaneous magnetization of the system will be positive; the other half will be negative equal time on an average. The consequences when we calculate a thermodynamic magnetization, average of different Monte Carlo Steps it will give zero, the system is magnetized.

But when we calculate the magnetization averaging over a large number of MCS, we are getting zero which is wrong, which is clearly a finite size artifact. So, then now of course, if we take larger and larger box sizes, the frequency of flips will decrease; but for larger and larger box sizes we also have to allow for the system to access different microstates, the number of microstates which are accessible also larger. So, we must average it better.

And if we really average it well, than any finite size systems there will be a finite probability for the system to go from positive to negative and negative to positive and you will get zero magnetization. It is only when the box size becomes nearly infinity, that you have an infinite energy barrier for the system to flip it is magnetic state from positive to negative at any finite temperature; the energy difference would be tending to

infinity between these high energy microstates and lower energy microstates. So, there is a very low probability or zero probability for the magnetic state of the system to flip.

So, what do we do? So, what is the problem? The problem is relatively high temperatures lower than T_c however; if we calculate the average magnetization naively, if you average over the Monte Carlo Steps there is a high probability that you will get zero magnetization whereas, actually the system is magnetized and how do we overcome this problem.

So, we should not simply go and start calculating average thermodynamic quantities, without understanding these subtleties; because doing it naively and brute force will give you wrong results, right ok. So, you know that temperature less than T_c , we do not know how to calculate T_c yet we will discuss it; but let us suppose we knew it, then we could get zero magnetization. However, at each Monte Carlo Step, if we calculated and averaged over the absolute value of magnetization, right; then we would get finite value of the average thermodynamic magnetization. Because independent whether the magnetization is positive or negative it will give a finite value, I mean it will give a nonzero positive value.

So, this is one solution, because that we take only the absolute positive value of the magnetization. But the problem will be, this will solve the problem that half of the time it is positive and half of the time it is negative; but what it will lead to is a finite value of magnetization, the average thermodynamic magnetization at T greater than T_c . Why is that? Because once the system has crossed the value of has a temperature greater than T_c ideally, half of the spin should be up and half of the spins should be down and on an average the magnetization will be zero and the magnetization will fluctuate about the zero value. Sometimes slightly positive above zero and sometimes slightly negative below zero; but when you average it, it should be zero right that is what it would be.

But now since we are always taking the absolute value, even at T greater than T_c we are going to get a finite value of the magnetization; and this is going to make it difficult to identify the transition temperature. So, in phase transitions, if you look up your statistical physics book; you would see that one identifies phase transitions to overcome such problems that we apply a small symmetry breaking B field, B for magnetic field specially at large box sizes.

So, what does this achieve? This achieves that one of those magnetic state, so B is a symmetry breaking field. It prefers suppose you apply it in the positive direction; then on an average the magnetic state where all the spins are pointing up will have a lower energy, so that and that magnetic state will be preferred. So, basically you are choosing, you are biasing one of the broken symmetry ground states of the system, you are biasing by applying this B field you are biasing one of the two ground states, without the B field equal.

So, whether the system is pointing up, most of the spins are pointing up or most of the spins are pointing down there is a symmetry in the system, both of the energies have the same energy; that is why it is able to go from positive to negative given enough for thermal large enough thermal fluctuations. However, if you apply a B field what happens is this, symmetry in the energy is broken by the application of this external b field and one of the ground states is preferred.

So, after that what you could take is the thermodynamic limit; so that the system cannot go from positive to negative and negative to positive. So, one of the micro one of the thermodynamic states is preferred, you take the thermodynamic limit, you will get a finite value of magnetization at T lower than T_c . And zero at or a slightly higher value above T greater at T greater than T_c and then you tend take the limit B tends to 0 to calculate the thermodynamic state.

We can also do that in simulations basically apply a small magnetic field to bias the system towards one of the ground states. Suppose you give a in the suppose you do your give the magnetic field in the positive direction; and then the positive, I mean the magnetic state where all the spins are up, pointing up will be preferred. Then you calculate the magnetization do your finite size scaling and do the analysis to figure out what will be the magnetization as N goes to infinity. Then do the same calculation for lower and lower B fields and basically extrapolate to calculate the magnetization and B equal to 0 or B tends to 0.

So, that is also possible, but for the purposes of the simulation which I shall demonstrate to you; I shall use this method and of course, it comes with artifacts we will try to understand the artifacts. Because you are choosing absolute value, then of course, it will be difficult for us to identify the transition temperature. Because you will have finite

magnetization at T greater than T_c ; however, we shall learn how to overcome it and find the transition temperature accurately.

So, till now what we have been doing is finding out, how the instantaneous magnetization varies with the box size at different temperatures, how does it fluctuate and so on so forth. Now, to calculate the phase diagram what we need is, basically to calculate quantities like the magnetization per spin, the average energy per spin or even the E square average; basically the energy of the entire system not per spin, the entire system E square is the energy square average or the magnetization square average, not calculated per spin as well as the entire magnetization of the entire box, the energy of the entire box.

And we shall need these quantities as we have discussed in our previous lecture; in one of our previous lectures to calculate the specific heat capacity or the heat capacity and magnetic susceptibility of the system. And these quantities shall prove very useful to understand how the transition temperature itself changes with the box size.

So, now our aim is to calculate the thermodynamic averages at different temperatures and plot these different quantities as a function of temperature. And see how these behave and this actually is the comparison with experiments which will tell us; because these are the quantities to calculate in statistical physics, you measure in the experimental lab and how well we do it depends upon how well the behavior of these quantities, the variation of these quantities with temperature match with the experimental system, alright.

So, basically what we have to do is, start at a high temperature or at a low temperature does not matter. We will start initially at higher temperature, any initial conditions say; random initial condition, equilibrate the system at that temperature, calculate these different thermodynamic quantities which will give us this and this and so on so forth. Measure this at a particular temperature, calculate the thermodynamic average; then slightly change the temperature, allow the system to reach equilibrium at that temperature in the new temperature.

Basically we have to equilibrate the system for say; N equal Monte Carlo Steps, we have to implement that in the code as well; and again measure these thermodynamic averages, again change the temperature, slightly measure these thermodynamic

quantities and keep writing these in a file. And at the end of our simulation so, we would have done it for suppose 15 or 20 different temperatures between say 3 and 1.5 or we can even increase the range; we have the thermodynamic quantities and we shall plot these quantities as a function of temperature.

Again we shall do finite size analysis; how do the transition temperatures change, how fine the temperature should we change temperature as a 0.1 or should it be 0.01 or should be 0.025; these are all questions which we have to try out and we shall try out on the computer. So, with this background let us go back and look at the code, I have already modified the code a bit.

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```

69 magw/=dfloat(N) ! Ni*L: magnetization (instantaneous) per spin.
70 !<math>M</math>
71 print *, 'initial energy E, E per spin =', E, E/dfloat(N)
72 print *, 'initial magnetization M, M per spin =', M, mag
73
74 ! INITIALIZATION COMPLETE.
75
76 open(10, file='ising_130_150_15_random_initial.dat')
77
78 do T_temp=30, 1, -1 ! TEMPERATURE LOOP
79
80   T = dfloat(T_temp)/10.000 ! FIX T
81
82   av_e=0.000; av_m=0.000
83   av_e_N = 0.000 ; av_e_N = 0.000 ! AV. E, M OF ENTIRE LATTICE
84   av_M2 = 0.000 ; av_M2 = 0.000 ! <math>\langle E^2 \rangle</math>, <math>\langle M^2 \rangle</math> OF ENTIRE LATTICE
85
86
87 do time=1, niter ! loop over no. of MCS
88
89   do m=1, 1 ! 1 MCS
90     do m=1, 1
91
92       call RANDOM_NUMBER(i) !<math>int(i) \in [1, N]</math> CHOOSING A LATTICE SITE.
93       call RANDOM_NUMBER(j) !<math>int(j) \in [1, N]</math>
94
95       n(i)=i; n(j)=j; n(i)=j ! Identifying neighbours of spin(i,j)
96       !<math>I \in \{i\pm 1, j\pm 1\}</math>
97
98       E1=-2.0*(log*float(spin(i,j))*spin(i,i)+spin(i,b,j)+spin(i,c)+spin(i,d)) ! BEFORE TRIAL FLIP
99       spin(i,j)=spin(i,j) ! TRIAL FLIP
100      E2=-2.0*(log*float(spin(i,j))*spin(i,i)+spin(i,b,j)+spin(i,c)+spin(i,d)) ! AFTER TRIAL FLIP
101
102      dE=E2-E1 ! DIFFERENCE IN ENERGIES.
103

```

So, the changes that I have done in this code is basically previously we had time equal to 1 to niter and the temperature was fixed at whatever value we would give, a we could change it, here I have introduced a temperature loop. Now, when you have a do loop the, you the variable in the do loop can change only as integer; so I cannot in Fortran 90 change the change these variables from say 3 2.9 2.8 and so on so forth. So, I have, I want to start at this temperature 3. So, I have multiplied this by 10, so that is 30, I want to stop at 1.5 temperature, I have multiplied it by 10 and to calculate the temperature I have divided this dummy variable T temp by a factor of 10.

So, as temperature change, so as this variable takes in value 30, 29, 28 and I have minus 1; so the value of T temp will decrease. Then when you divide it by 10, you get values of

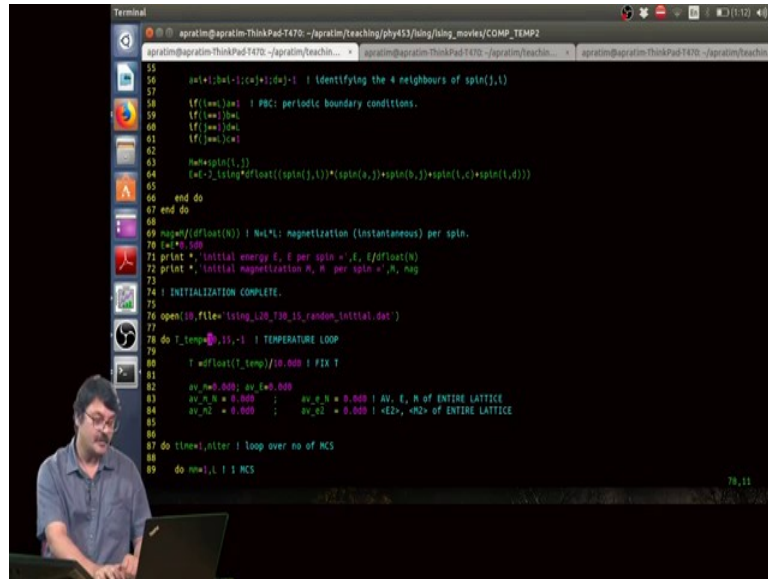
T to be 2.9, 2.8, 2.7, 2.6 and so on so forth. So, the value of this temperature will vary from 3 to 1.5 right I have to keep this quantity an integer, these quantities I have already defined at the beginning of the code.

So, I will be discussing various values or the calculation of different quantities in the code, but I have in the not in the class, but otherwise changed the values and defined those values as real or integer quantities. The other change that I have done is, I have made all these real quantities, they were real when were being introduced. I was introducing you the code I have converted into real star 8. Real star 8; means that these variables are accurate up to 16 places of decimal, right. So, number of significant digits has increased.

The other thing that I have done is, I basically change various parameters, lattice size, sometimes I shall go from low temperature to high temperature, high temperature to low temperature; however, I shall always start with a random initial condition. As I told you the final thermodynamic state of the system does not depend upon your initial configuration; however, later we shall see some artifacts, specially at lower temperatures, if we start from lower temperatures, but we will discuss that later.

So, what we have here is the initial condition; then I basically calculate the initial magnetization and energy of the entire lattice this is exactly as before. And then here we calculate the magnetization per spin, the energy per spin and printed this is exactly as before; here I have introduced a new loop over temperature, which goes from 3 to 1.5.

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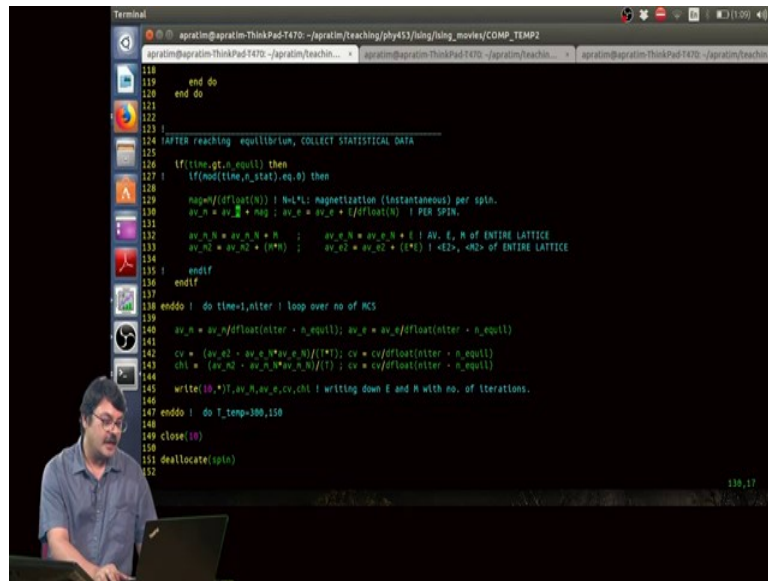


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In addition at each of these temperatures we have to calculate the average energy, the average magnetization, e square average, m square average and these quantities at each temperature have been initialized to 0.

Why have been, they initialized to 0 these average quantities? Because at each temperature, I am going to add the instantaneous value of e square, the instantaneous value of energy, the instantaneous value of magnetization to these variables keep on adding it as we go over different Monte Carlo Steps. And the end, at the end of calculating the average at each temperature I shall write it down. So, I have introduced.

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```
118     end do
119   end do
120
121
122
123
124 !AFTER REACHING EQUILIBRIUM, COLLECT STATISTICAL DATA
125
126 ! If (time.gt.n_equal) then
127 !   If(mod(time,n_equal).eq.0) then
128
129   magm/(dfloat(N)) ! M=L: magnetization (instantaneous) per spin.
130   av_m = av_m + mag ; av_e = av_e + (dfloat(N))-1 PER SPIN.
131
132   av_e_N = av_e_N + E ; av_e_N = av_e_N + E ! Av. E, N of ENTIRE LATTICE
133   av_e2 = av_e2 + (E**2) ; av_e2 = av_e2 + (E**2) ! <E>, <E^2> of ENTIRE LATTICE
134
135 !   endif
136   endif
137
138 enddo ! do time=1,niter ! loop over no. of MCS
139
140 av_m = av_m/dfloat(n_iter - n_equal) ; av_e = av_e/dfloat(n_iter - n_equal)
141
142 cv = (av_e2 - av_e**2)*N/(T) ; cv = cv/dfloat(n_iter - n_equal)
143 ch1 = (av_e2 - av_e**2)*N/(T) ; cv = cv/dfloat(n_iter - n_equal)
144
145 write(*,*)T,av_m,av_e,cv,ch1 ! writing down E and N with no. of iterations.
146
147 enddo ! do T=temp=100,150
148
149 close(10)
150
151 deallocate(spin)
152
```

So, at each temperature, you have the end of the do loop over time, a time goes from 1 to niter, right. And so, here is where we calculate the different average of these quantities, I am adding average m the to magnetization to the quantity average m, energy per spin to average e and so on so forth. And after a certain number of Monte Carlo Steps at each temperature, I am calculating the thermodynamic averages. Now, we have calculated it over you have added it over and over again, over a certain number of Monte Carlo Steps, so you have to divide by it, right.

So, that you get the average thermodynamic state of the system. So, that is being done here and here is the end of the loop of temperature. Now, one more thing as I told you, when we were working on the screen is basically at each temperature you have to allow for the system to reach equilibrium. So, when you choose. So, here is at each at a particular value of temperature time goes from 1 to niter, but over n equal ah. So, n equal for number of Monte Carlo Steps you allow the system to equilibrate at each temperature only when time is greater than n equal right. Basically you start collecting data to calculate thermodynamic averages .

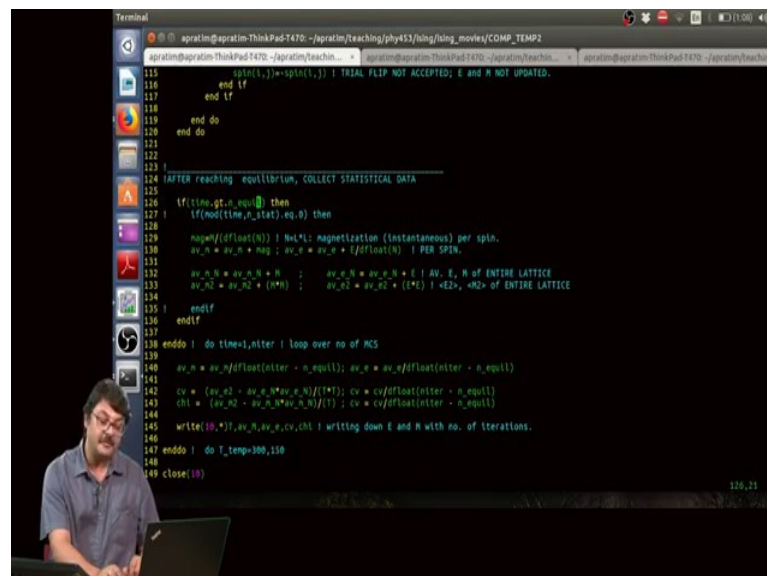
So, at each temperature time goes from 1 to niter; however, niter should be such. So, niter should be always greater than n equal number of iterations you allow the system to equilibrate; one has to be careful while giving the value of niter. And after, suppose you choose n equal to be 10000 iterations that is exactly what I have done here, right at the

beginning of the code; where I define various variables where I choose the lattice size and the number of iterations, etc; it is there that I set n equal to 10000.

Now, you would have remembered that even for relatively large lattice sizes L equal to around 60 cross 60 and 80 cross 80 you were needed around 2500 iterations for the system to reach equilibrium. At higher temperature the system will relax to equilibrium even faster, but then why have I chosen n equal to be 10000 iterations? Because when we were analyzing the data, when we were looking at relaxation to equilibrium, we were primarily looking at relatively higher temperatures as you go down in temperature 1.5 and 1 and so on so forth, even lower temperatures.

The time that the system takes to reach equilibrium, before we can start taking thermodynamic data or statistical data to calculate thermodynamic averages is even higher. You can explicitly check how much time it takes for the system to reach equilibrium at lower temperatures. I have here taken it to be 10000 iterations for safety. But at very lower temperature you might even take much higher number of iterations for the system to reach equilibrium; however, for 1.5 10000 iteration temperature of 1.5 10000 iterations is enough.

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```
115 spin(i,j)=spin(i,j) ! TRIAL FLIP NOT ACCEPTED; E and N NOT UPDATED.
116 end if
117 end if
118 end do
119 end do
120 end do
121
122 !
123 !
124 !AFTER reaching equilibrium, COLLECT STATISTICAL DATA
125 !
126 !f (time.gt.n equil) then
127 ! f(mod(time,n_stat).eq.0) then
128
129 magnetization (instantaneous) per spin.
130 av_n = av_n + mag ; av_e = av_e + E/float(N) ! PER SPIN.
131
132 av_n2 = av_n2 + N ; av_e2 = av_e2 + E ! AV. E, N of ENTIRE LATTICE
133 av_n2 = av_n2 + (N*N) ; av_e2 = av_e2 + (E*E) ! <E>, <E^2> of ENTIRE LATTICE
134
135 ! endif
136 !
137 !
138 enddo ! do time=1,niter ! loop over no of MCS
139
140 av_n = av_n/float(niter - n equil); av_e = av_e/float(niter - n equil)
141
142 cv = (av_e2 - av_e*av_e*N)/float(N); cv = cv/float(niter - n equil)
143 ch1 = (av_n2 - av_n*av_n*N)/float(N); cv = cv/float(niter - n equil)
144
145 write(10,*) av_n, av_e, cv, ch1 ! writing down E and N with no. of iterations.
146
147 enddo ! do T_temp=100,110
148
149 close(10)
```

And only when time is above 10000, do we start taking data for calculating thermodynamic averages. And when we calculate the average magnetization or the average energy of the system; we suitably divide it because we are adding it over

different Monte Carlo Steps, we suitably divide it by niter minus n equal. We are, if we are collecting data every Monte Carlo Steps as the system accesses different micro-states, then we should divide it suitably by the number of micro states over which we have collected data.

The other thing which I have not implemented, I mean I have implemented and commented it out is; it is often not necessary that you calculate thermodynamic or you collect statistical data to calculate thermodynamic averages at every Monte Carlo Step. The when you collect data, these different micro-states have to be statistically independent; they have to be changed significantly.

Now, at higher temperatures it does change and that is why I have collected data to calculate thermodynamic averages every MCS. However, depending upon the problem in question you might want to calculate different thermodynamic quantities or collect data to calculate different thermodynamic quantities after every n stat step.

So, you do not calculate collect data every Monte Carlo Step. But suppose n stat is 10 or 20 or the time it takes for the system to relax to a new micro-state. So, only, so if you have this relation, if mod time n stat equal to 0; so if n stat equal to 10 mod time comma n stat will be 0 every 10 iterations. And if you have these, if you include this line in the code of course, with a suitable 'endif'; then you are collecting data every 10 steps if n stat is 10 and suitably you have to then also while calculating the average you have to multiply the denominator by 10 .

With this background, so here I have basically discussed how the code has been changed, what modifications you need to put include in the code to calculate thermodynamic averages. So, in the next class we shall actually look at the data, various thermodynamic quantities as a function of temperature and analyze it as a function of different lattice sizes and see what we can understand about the system. Or even before identifying the so, called critical point the temperature at which the system goes undergoes a ferromagnetic to paramagnetic transition or vice versa.

If you are going down in temperature, what are the things to be aware of in terms of simulations, what other artifacts could creep in, before we reach our final answer. Understanding these little details are extremely important to do a simulation correctly;

writing the code will give you some result, but it could well be junk. And so, unless you understand these various artifacts even with the correct code one could get wrong data.

Thank you.