Computational Physics
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Lecture - 21
Monte Carlo Simulation Analysis
Part 01

Welcome back, what I am going to start with today is having a quick recap of what we discussed in the last classes.

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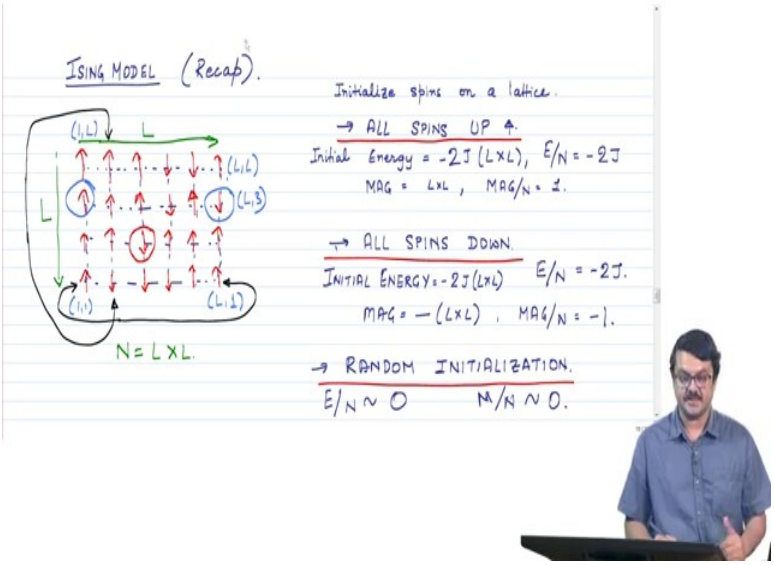

We were discussing Ising model, in which there are spins on a lattice which can either point up or down, which are interacting with…. any spin is interacting with it is neighbors with the Ising Hamiltonian which is minus J sum over S i dot S j where any spin interacts with it is nearest neighbors; which in a 2 D case is just 4 nearest neighbors. The size of the lattice was given by L and then the total number of spins is L cross L in a 2 dimensional lattice; if you have a 3 dimensional lattice then the total number of spins will be L cross L cross L.

In the last class, we discussed about initializing the spin on the lattice. So, you can initialize the spins, where all the spins are basically pointing up; in that case, that the initial energy. So, all this right, even before starting the Monte Carlo iterations

simulations you are going to basically initialize all the spins; you can do it as up or down or even you could have a random initial condition. If you have a, if you start with all the spins up then the total initial energy of the system will be minus 2 J L cross L right; L cross L being the number of spins in the lattice.

The energy per spin will be minus 2 J right, the magnetization will be L cross L and magnetization per spin will be plus 1 because all the spins are pointing up. So, magnetization per spin is plus 1; magnetization is simply the sum of all the spins in the lattice the value of the spins in the lattice. If you have all spins down, then the initial energy again will be 2 J into L cross L, because 2 spins pointing up or 2 spins pointing down, they have the same value of the energy. The energy per spin again will be minus 2 J just as here, but the magnetization per spin; however, will be minus 1.

So, if you get these values right, then at least your calculation of the energies is going right; so this is a quick check. However, if you can also start with random initial condition and then the initial energy; so half of the spins are pointing up, half of the spins are pointing down on an average, any spin will have 2 neighbors which are pointing up 2 neighbors which are pointing down. In that case the energy per site you know the energy per spin would be some number close to 0, it will not be exactly 0 and the magnetization will again also be some number close to 0.

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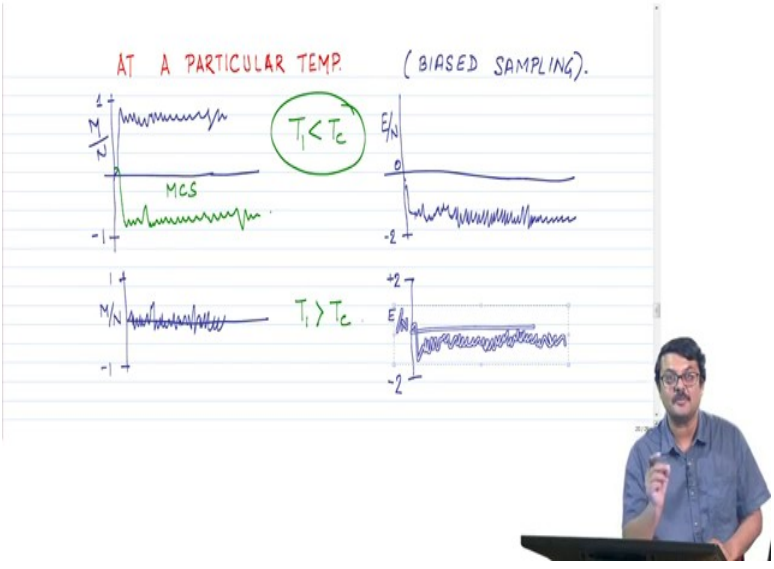

Then what we did in the last class is, perform Monte Carlo simulations using the metropolis algorithm. Basically what we are doing is, calculating a spin flip, having a trial spin flip, calculating the energy of the lattice before and after the spin flip. And, if the spin flip decreases the energy of the lattice, then you accept the spin flip, the magnetization changes and this is a biased sampling. The metropolis algorithm is a biased sampling, because any higher energy microstate is accessed with the probability E to the power delta E by K B T.

Or rather flip due to the spin flip, if the microstate has a higher energy as a consequence of the spin flip, then that microstate or that attempt is accepted with probability E to the power minus delta E by K B T right. So, what we did in the last class is also plot the magnetization versus number of Monte Carlo steps and it was fluctuating about a certain value some value close to plus 1. If the temperature of the system was less than T c, the critical temperature and if you were starting from a random initial condition, initial magnetization would be 0. But it would go up and fluctuate about some average value.

Also, if you had a different sequence of random number seeds, it is also possible that the magnetization goes down and fluctuates to a value close to minus 1; because all spins are, nearly all spins pointing up and nearly all spins pointing down have an equal value of the energy. So, both the microstates which are all spins pointing up or all spins or nearly all spins pointing down have the same probability right. The energy would fluctuate around just some value above minus 2, if you are in a magnetized state that is T 1 is less than T c.

However, if you chose temperatures which are higher than T c then the magnetization fluctuates about 0 right, that is what we saw. And the energy, the value of the energy also of the system also goes to a higher value than minus 2, right; it also fluctuates to about some value close to 0. So, when I am plotting this energy and the magnetization; of course, I am talking about the instantaneous magnetization, the magnetization of a particular microstate not the thermodynamic magnetization.

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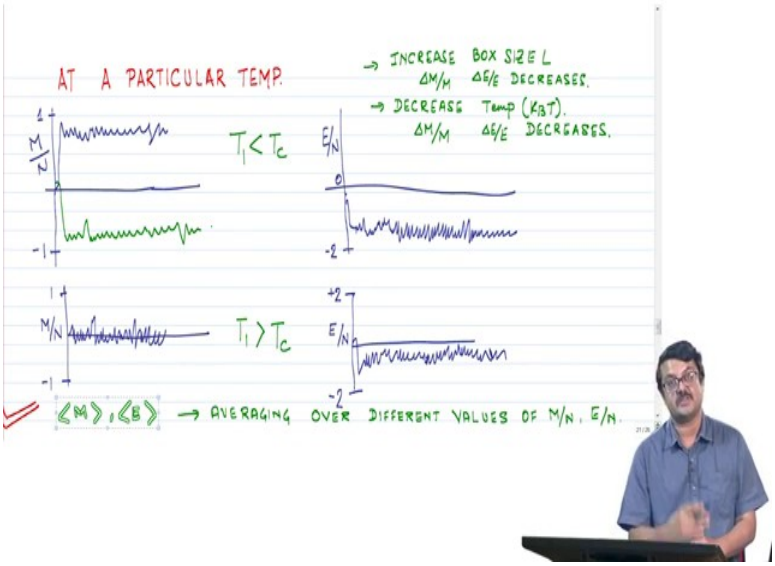

But that, the thermodynamic magnetization which statistical physics deals with, is basically the average magnetization over all these different microstates right. So, basically M and E, so average magnetization of the average energy can be calculated by basically taking the values of these magnetization of instantaneous magnetization at each of these microstates and averaging them over.

So, basically you have magnetization the instantaneous value of M at after 1 Monte Carlo step, after the 2nd Monte Carlo step, after the 3rd Monte Carlo step and just average them over a large number of Monte Carlo steps and then you have the average magnetization E and M. So that is the principle; but of course, just reminding you the system will have a relaxation time. So, if you are starting from the initial condition, you should first allow the system to equilibrate and then calculate start calculating these quantities.

We also saw, that if we increase the box size then the fluctuation in the magnetization or the fluctuation in the energy decreases. You have larger number of spins, since the fluctuation decreases furthermore; if you decrease temperature right, then also the fluctuation in the magnetization and fluctuation in the energy decreases. That is what temperature does, temperature basically gives fluctuations to the energy, hence to the magnetization.

So, if you remember your canonical ensemble statistical physics, you basically the system takes energy from a external heat bath or gives energy to the external heat bath. As a consequence of which, the system is able to access different microstates of different energies and that is exactly what we are doing in our Monte Carlo simulation of the Ising Model. Except we do not have an explicit heat bath, I mean we have not modeled it explicitly; but we are taking in energy, we are giving out energy, right.

So, that seems quite simple, because you can now have access to those so called thermodynamic quantities and that is what the phases are that the experimentalist is interested in?

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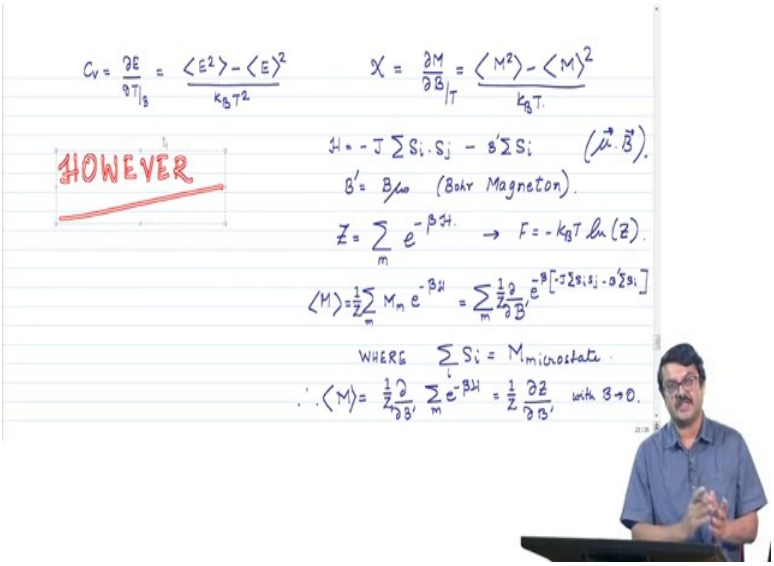

And one can also calculate the specific heat capacity which is del E by del T at a constant B at no magnetic field say or a constant magnetic field. And you can see in statistical physics and I think I discussed in one of the previous classes, that C v which is del E del T, the amount of change in energy of the system due to a change in temperature is related to E square average. Which is the average energy of the system not per particle of the entire system E square average minus E average square which is nothing, but the variance; it is nothing, but the variance of energy divided by K B T square right. And you can just look that up.

So, basically the specific heat is related to the fluctuation in energy divided by K B T square. And you can see that the dimensions del E del T, so it has dimensions of energy

per temperature; and here you have dimensions of E square energy square and you divided by K B T that is dimensions of energy and then there is an extra T. So, the dimensions match right. So, if you calculate C v, just like you calculate the value of this quantity E square average minus E average square. So, this basically this angular arrows are of course by calculating the value of E square at different microstates as you go on doing the Monte Carlo simulations.

At the end of every Monte Carlo Step you can calculate the value of E square right; and then take an average E average you can of course, take when you can calculate the total average of basically average the energy over the entire number of Monte Carlo simulations; then you get C v. Similarly you can calculate susceptibility chi which is nothing, but del M del B; del M means when you switch on a magnetic field and so, there is a slight perturbation in the magnetic field B; then how much is the change in magnetization; that is what the susceptibility chi measures.

And one can check the basically chi is related to M square average minus N average square by K B T. So, M square average minus N average square is nothing, but the variance in magnetization, right. So, this is the variance, expression for the variance. One point, till now when we wrote down the Ising Hamiltonian there was no B, no magnetic field B, right. So, where does susceptibility come from?

So, basically and how can you calculate susceptibility just by using the variance. Just to give you an idea and so, the Hamiltonian H was minus J S i dot S j sum over all spins right and you can also add a term which is nothing, but minus mu dot B; mu being the magnetic moment of each spin into B, B being the magnetic field. And here since we are writing in terms of essentially the spin, where basically mu is nothing, but the Bohr Magneton multiplied by the spin.

So, hence I have written instead of magnetic field, I have written at B dash where B dash is nothing, but the magnetic field B into the Bohr Magneton. So, you can also write it like this, and then in this case the partition function Z will be e to the power minus beta s sum over all possible microstates, the free energy is of course, minus K B T lon of Z. And the average magnetization right, can be written as the M subscript small m which means basically the instantaneous magnetization, the magnetization at each microstate; the average magnetization is basically sum over all possible accessible microstates the

magnetization of that microstate the instantaneous magnetization of that micro straight into e to the power minus beta Hamiltonian energy, right.

And this can be written as basically as some overall microstates here minus del del B dash, B dash being the magnetic field expressed in terms of Bohr Magneton. So, this rescale magnetic field del del B dash into minus e to the power minus beta, beta 1 by K B T minus J i minus J S i dot S j summation minus B dash summation S i right. So, basically where, if you take a derivative with respect to B dash, basically this sum of S i will come down in the denominator right this is an exponential function. And sum over S I, the total sum of all the spins in the lattice, is nothing but the magnetization of that microstate, right.

So, basically then the average magnetization in statistical physics can be written as minus del del B dash into Z, which is derivative of the partition function with respect to B dash or the magnetic field; and later we can take B tends to 0 right. So, hence what is the point? The point is, basically even though you do not have an explicit magnetic field in the system or you are not modeling that explicitly when we wrote our code; you can get the chi susceptibility right. Even in the absence of magnetic field, calculating it from equilibrium properties right; it is related to the M square.

You can just check that M square minus M average square it will be nothing, but double del M del B; you can carry this step out for once more right. You take the derivative of this quantity with respect to B and you can get M square minus M average square by K B T, because you will also have a beta factor there right; the beta will also come down which I have not written here, but you can fill that in. So, in principle basically if you are able to generate different microstates, then you can calculate M, average M, average E, C v, chi over these different microstates which we generate in a computer and we can compute all the properties of the system.

We can also basically calculate these quantities as a function of temperature and then basically study the phase diagram of the system. However,; before you complete; however, before you start calculating these things there are some other issues or artifacts of simulations to be aware of; and only after fully understanding those issues should one start calculating the average magnetization the average C v high and so on so forth. So, let us move to the computer and see the data and let us learn a bit more about the artifacts

before coming back to the physics and calculating C v, chi, M as a function of temperature.

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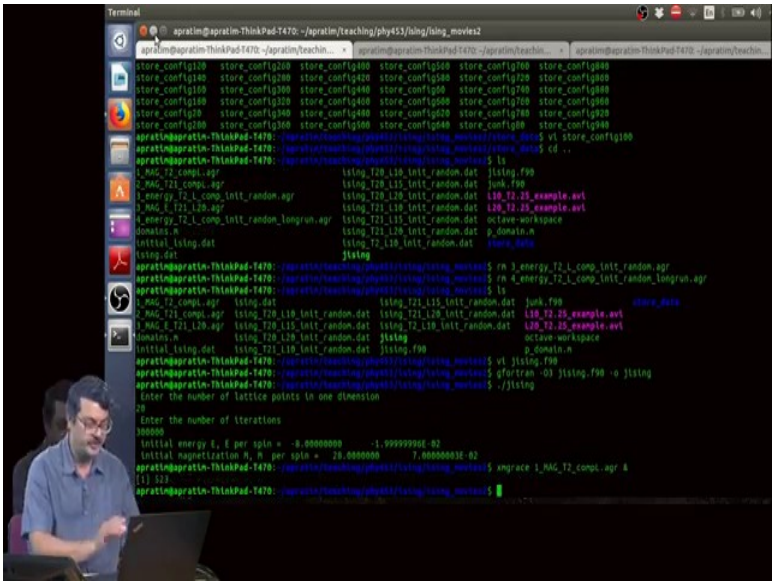

So, looking at the code again v i J Ising dot f 90.

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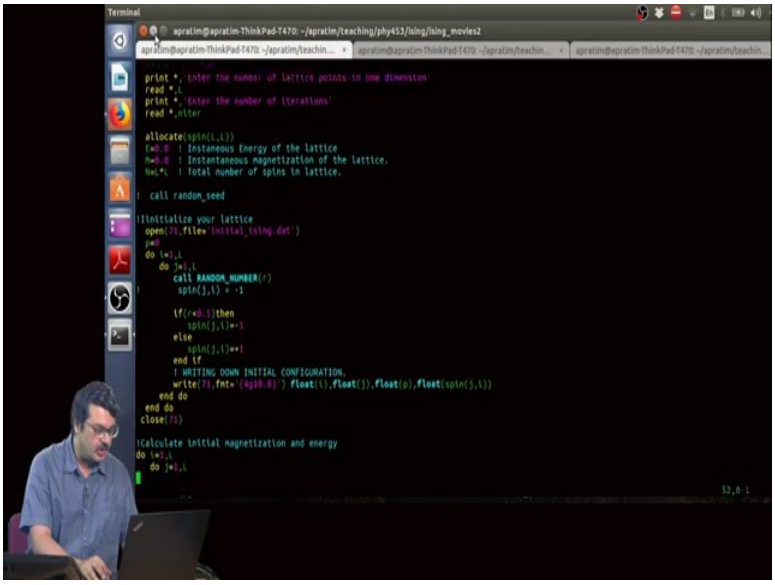

What we want to do right now, is basically plot magnetization energy versus Monte Carlo Steps (MCS) for slightly smaller box sizes. So, we already did it for box size 40 and 60 and 80 in the last time and we saw all the energy fluctuations; but if we have slightly smaller box sizes box of 10, 15, 20, let us see if we see something strange or

unexpected when we plot the magnetization versus MCS. So, all that I am doing here is basically I am going to run the data at temperature T equal to 2 box size is equal to 20 all right and all the data which is basically the time.

Here is the time the magnetization per spin and the energy per spin is going to be written down in this file, just as previous times right. So, g fortran minus 0 3 jising dot f 90 minus o jising, compile and jising I am going to run the code 20; temperature is already given as 2 in the code just as we did it last time and suppose we have 300000 iterations. Now, I have already done the simulations for different box sizes and what I shall do is basically just show you the data, I have plotted it ok.

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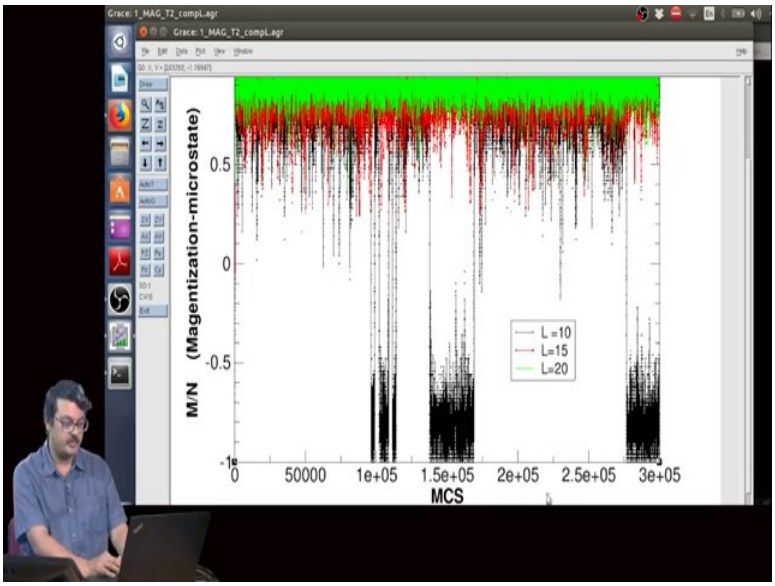

So, this 2 D Ising model and basically I am plotting magnetization per spin versus MCS the Monte Carlo Step and I have showing the data for 300000 iterations right. Now the black data is for L, the lattice size equal to L equal to 10, so you have 100 spins in the lattice. The red data is for L equal to 15 and the green L is for 20.

Now there is something which you did not see last time, when you have L equal to 10 starting from a random initial condition the spin, the magnetization, the instantaneous magnetization essentially went up some number close to plus 1. But after fluctuating for some time, you see that the magnetization has gone from some number close to plus 1 to minus 1. And then here it goes up again and comes down again and here there is a gap

and here again it goes up to plus 1 and here again it fluctuates about minus 1; of course, the average energy in these two states either close to plus 1 or minus 1 is the same, right.

So, but previously we saw that the energy was going up or down and sticking and fluctuating about some average value. But here we see that the state of the system is going from plus M to minus M. Now if you just took an average for L cross for L equal to 10, if you average the magnetization over a long run right; in the previous cases you would get a constant value, but here since sometimes it is plus 1 close to plus 1 and sometimes is close to minus 1, if you take a good average you will get a 0. So, why is this happening?

So, this is the question whereas; for larger lattices L equal to 15 or L equal to 20 you see it is fluctuating about some average, value just as seen it previously. Now the L equal to 10 case is a bit strange. So, let us try to see what happens, when you increase the temperature slightly. So, I have already done that and here is the data for L equal to 10 up to 300000 iterations ok; a Monte Carlo Steps equal to 300000 and the number of iterations at temperature of 2.1.

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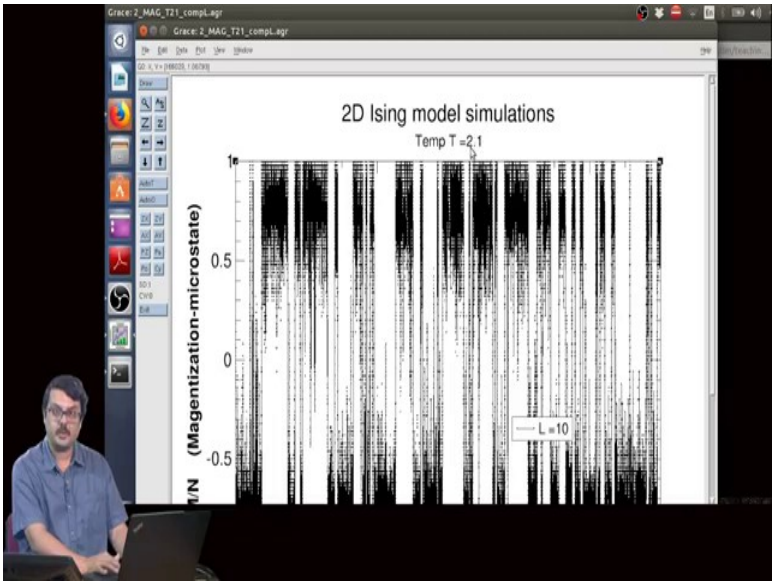

And here we see when we increase the temperature to 2.1, there are rapid flips where the magnetization of the L equal to 10 lattice goes from plus from plus to minus back to plus back to minus and so on so forth; it becomes much more frequent. What about L equal to 15 and L equal to 20, so I have already plotted it, I will just switch it on. So, when you

go to L equal to 15, again now at a slightly higher temperature the spin goes from minus 1 to plus 1 again back to minus 1 again to plus 1; but for a higher the size of the lattice this jump from plus 1 to minus 1 becomes less frequent .

With the increase in temperature the frequency increased; but as you increase the lattice size the jump from plus 1 to minus 1 is less frequent. If you remember for L equal to 80, L equal to 60 or 100000 iterations we hardly saw such behavior. Now this is very odd and fishy, because if you have a magnet right; so what is this plus 1 to minus 1 mean, basically the magnetic state is flipping.

So, if you take a real magnet, if you keep it suppose the North Pole is pointing in this direction in the morning, you do not come back in the evening; and say see that the North Pole has become in the opposite direction the North Pole and the South Pole does not flip right. So, the magnetic state is it is either plus 1 or minus 1 is basically saying that the direction of the magnetization and it does not flip really. So, why is this happening? So, this is a finite size artifact.

So, let us explore this in a bit more detail, because unless we understand what is happening here and we take a naive average we will get 0 magnetization; if you average over all microstates especially at temperatures close to T c when you see such large flips happening. And the you will get 0, because half of the time the system is in the plus state, half of the time it is in minus state; magnetization the magnetic state is still not, it is not unmagnetized, it is either plus 1 or minus 1.

If you take the average you will get a 0, which is an erroneous value, why is this happening and how do we overcome such issues; to understand that let us look at what the spins are doing more explicitly ok. So, what I am going to do is, basically may show you a movie of where I explicitly follow each spin as a function of time; and the way I do it is basically I have some commented out statements, I comment them in.

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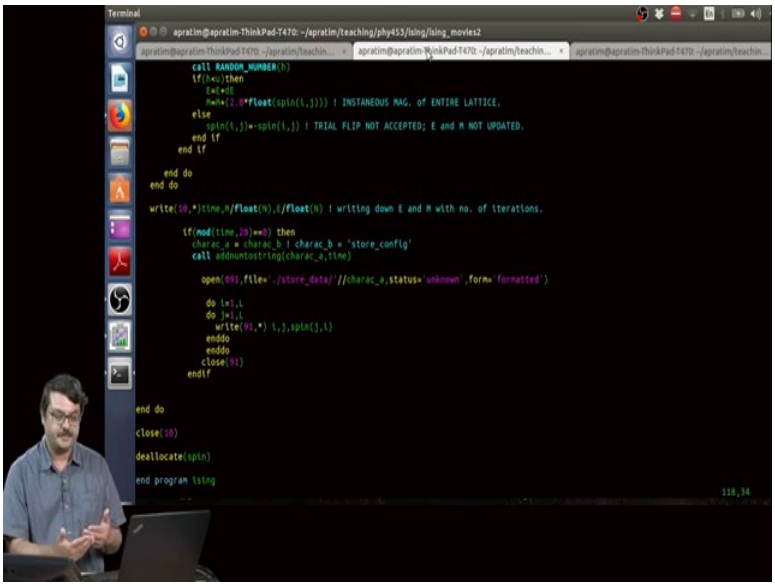

So, here all that is being done in these steps is, after every around 20 Monte Carlo Steps I am writing down i equal to 1 to L, j equal to 1 to L. So, I am going to each point in the lattice and writing down the coordinates; i and j are the coordinates of that lattice point and the value of the spin at that lattice point.

So, what is happening is after every 20 steps I shall explicitly get to see, what is the spin state right. We are already calculating that, but here we can follow each and individual spin. And we write down the microstate the position of each spin in file, right; and what I am going to do is then make a movie file and see it, so that we can follow it.

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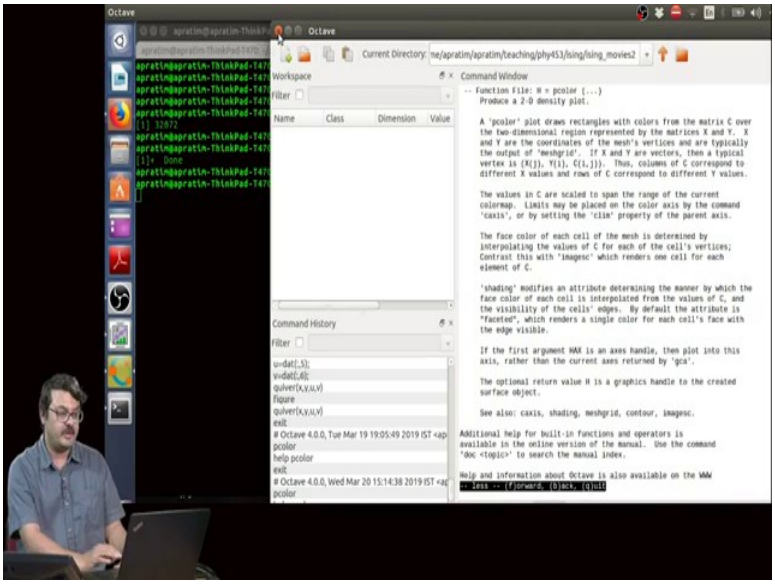

To make the movie file you can use the software called Octave, it is equivalent to the MATLAB except that Octave is free, is freely downloadable. And I am going to use the command called p color to basically plot all the data. So, I have already done that and you can learn this on your own if you want by reading about p color and reading about octave. But what I am going to focus is I have already saved the positions of all the spins every 20 iterations in some file; and I am going to basically show you the movie about the state of those spins.

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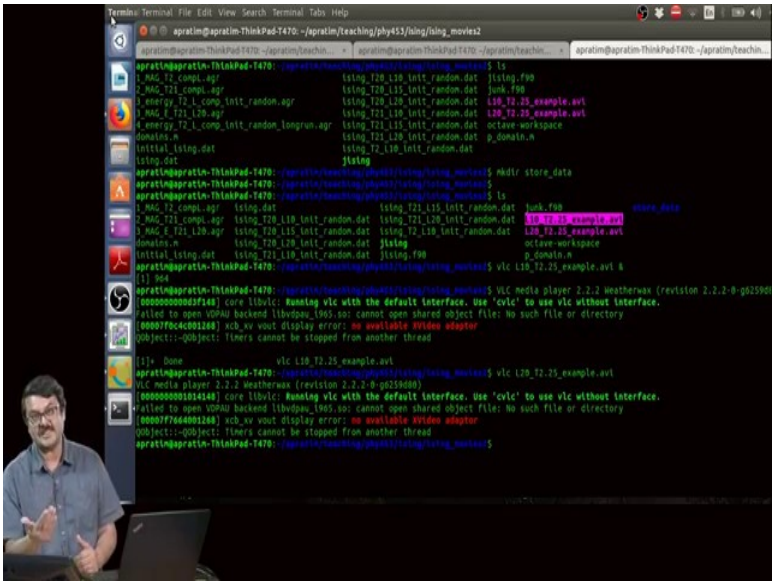

So, this is for a 10 cross 10 lattice at temperature of 2.25 and let us see what happened?

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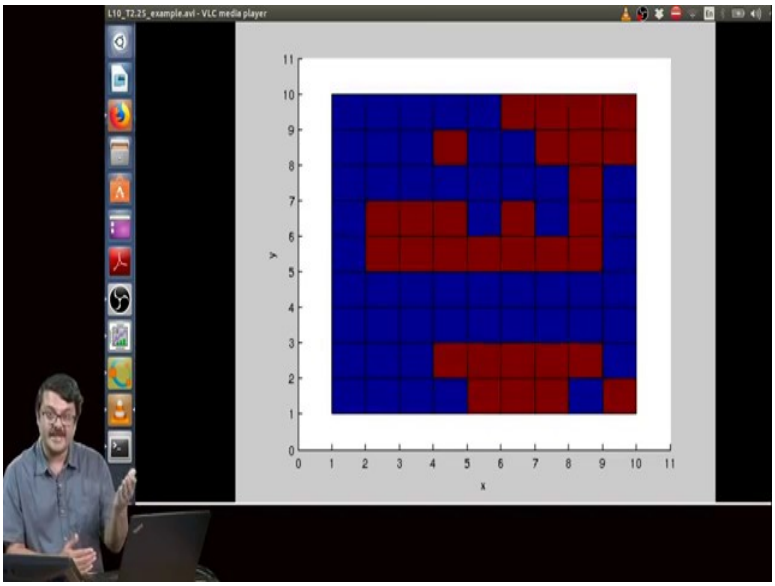

So, just to stop it, let us suppose here you see that the entire lattice, blue suppose stands for spins pointing up; red stands for spins pointing down. At temperature of 2.25 you see most of the spins are pointing up and 3 spins are pointing down. So, basically the magnetic state is plus 1, some number very close to plus 1.

But as we evolve the system through Monte Carlo Steps you see that there are fluctuations right, and suddenly the entire state of the system has changed where all the spins are pointing up. So, these are these red colors have basic sorry they are pointing down, red was corresponding to spins pointing down in a few, only a few spins are pointing up. So, basically the magnetization has gone from a state which is close to plus 1 to close to minus 1 and we see that all the spins are going either up to down and down to up rather frequently, right.

So, here you are able to follow each spin and different microstates; this is basically an explicit representation of the microstates right. And, we see rapid changes in the magnetic state of the system from plus 1 to minus 1 as we change. Now, for a larger lattice you have 20 cross 20 lattice sites. Again let us say blue corresponds to spins pointing up; red corresponds to spins pointing down. And here you see that the, you have these fluctuations some spins are pointing up and down; but on the large times most of the spins were pointing blue. But after a considerable amount of time it has changed to red.

So, again that is what we saw in the graphs also, right; the spins by going from plus m 2 minus m. But for a larger lattice as you saw explicitly in the movie, the changes from plus 1 to minus 1 or minus 1 to plus 1 is less frequent.