

Computational Physics
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Lecture - 18
Monte Carlo Simulation Algorithm & Implementation
Part 01

Welcome to the second class of this module, where we shall discuss Monte Carlo algorithm in much more detail, so that by the end of today's class you shall be able to write down a simple Monte Carlo algorithm on the computer and be able to model the Ising model.

(Refer Slide Time: 00:20)

MONTE CARLO ALGORITHM (IN DETAILS)

BROAD FLOWCHART →

- ① INITIALIZE LATTICE.
- ② EQUILIBRATION AT A PARTICULAR T
- ③ GENERATE MICROSTATES AT A PARTICULAR T .
 $N_{MCS} \rightarrow$ CANONICAL ENSEMBLE
- ④ CALCULATE THERMODYNAMIC QUANTITIES.
 $\langle E \rangle, \langle M \rangle, \langle C_V \rangle, \langle X \rangle$.
 $\langle E \rangle = \frac{\sum_k E_k e^{-\beta E_k}}{Z}$ SO $\langle E \rangle = \frac{\sum E_k}{N_{MCS}}$
- ⑤ CHANGE TEMPERATURE T
- ⑥ PLOT AND MONITOR $\langle \rangle$ QUANTITIES WITH T .
 \rightarrow DO PHYSICS.

BIASED MONTE CARLO
 BUT METROPOLIS ALSO
 ACCESSES STATES WITH
 PROB $e^{-\beta E_i/2}$

Before I go on, in today's class let me give you a 2 minute recap of what we discussed in the last class. In the last class we discussed that we are going to learn about Monte Carlo simulations and in particular model the Ising model. And implement it on the computer, and look at the change in the magnetization of a lattice of, a lattice of atoms as a function of temperature and through that we basically understand the ferromagnetic transition from such that a magnet which is in a magnetic state at low temperatures goes through the disordered state at higher temperatures.

So, we have Ising model is essentially a microscopic model to describe this phenomena. And using statistical mechanics, and using model of this one can basically monitor the thermodynamic quantities like energy, magnetization, specific heat capacity, and chi, the susceptibility chi, as a function of temperature and at the transition temperature which is T_C , the critical temperature at which the ferromagnetic to paramagnetic transition occurs.

These quantities show a certain change in behaviour, basically the order parameter magnetization goes to 0 and that is how we characterize the so called critical temperature T_C and chi show other properties, they will show peaks. But we shall discuss this in greater details. The question is how do we model all this physics, all the statistical physics on the computer.

A primary question is also that why do we need to model all such stuff in the computer. The Ising model can be exactly solved analytically in 1D and 2D. So, let me tell you what does it mean by solving the Ising model in 2D. It means that you can calculate the partition function using statistical physics you can if you calculate this partition function, you know that all of the thermodynamic quantities can easily be calculated from by taking suitable derivatives of the partition function, that is what we discussed last time, right.

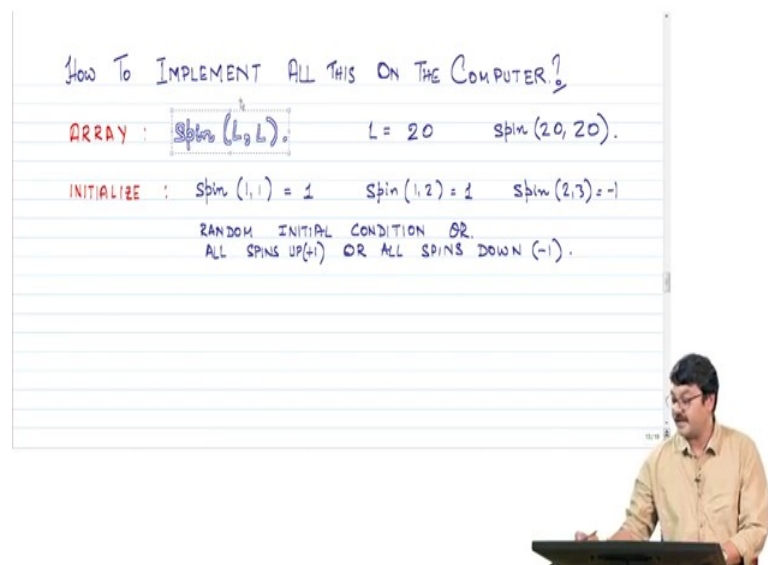
Now, if you have the Ising model Hamiltonian you can exactly calculate the partition function on circuit they did it way back in the 1930s or 40s and you can exactly calculate C_v , E , M all the thermodynamic quantities as a function of temperature and, so you can essentially understand how the Ising model behaves. You might already have done a mean field version of magnetic transitions for magnetic transitions in your statistical mechanics class, but a simple model, as simple as Ising model where you basically have a spin which is interacting with just its neighbours, just as 4 neighbours in 2D and maybe 6 neighbours in 3D if you have a cubic lattice.

In 3D the Ising model is not solvable till date. You can only do it either using extreme on the computer or extremely advanced analytical techniques which where also you will get you will need approximations, ok. So, just as, so the point I want to say emphasize on is that of course, you can exactly calculate the partition function of an ideal gas, you can calculate the partition function of an Ising model in 1D and 2D exactly. But as soon as

you go to slightly more complicated Hamiltonians interaction systems you often need the help of computers to be able to exactly understand, which means calculate the thermodynamic properties you know and relate it to the thermodynamic physics you need the help of the computer, you cannot do it exactly, more often than not, ok.

And through this calculation you are basically trying to understand how you are going to do it, how you are going to do Monte Carlo simulations far more complicated Hamiltonians with. So, Ising model is basically one of the simplest Hamiltonians if you understand that how to implement that. The principles of calculations remain the same. Other complexities due to the Hamiltonian increases, ok. So, with that background let us get down to actually discussing what is the broad flowchart or what is the algorithm in basically modeling the Ising model on the computer.

(Refer Slide Time: 06:07)



So, what we need to know, as you know, as we discussed last time that basically spins on a lattice can be described by; I will just remind you an array a two-dimensional array of L cross L, L being the size of the lattice.

And what one has to do is basically at the beginning initialize the lattice, which means give values to these different elements of this array as plus 1, minus 1, whatever you whatever be the you want the whatever way you want to initialize the lattice. Of course, your final thermodynamic state does not depend upon your initial state. So, after

initializing a lattice you have to equilibrate your lattice or your system which your model on the computer for a particular temperature.

So, you have to reach the equilibration (Refer Time: 06:59) to basically you have to do a few Monte Carlo steps of your system, so you have a few iterations of your system where you evolve the system, so that the system first reaches equilibrium. And once it has reached equilibrium what you are doing essentially you are generating different microstates of the system on the computer.

So, the system is accessing different microstates and basically in the Ising model as per the algorithm that we discussed in the last class, you are essentially modelling or you are using the canonical ensemble description of the Ising model on the computer. Why? Because energy can fluctuate; basically, the energy of the lattice can increase. When there is a spin flip happening, it could either the total energy of the system could either increase or it is possible that it could decrease in which it is giving away energy to a bath essentially all right.

And while generating, so once you have reached equilibrium you can have basically N MCS, N for the number of Monte Carlo steps, at a particular temperature where the system accesses different microstates and as the system accesses these different various microstates you can use those to calculate different thermodynamic quantities. Thermodynamic quantities like the average energy say, or the average magnetization or the average C_v being the specific heat capacity or the susceptibility, the average values. These are averaged over these angular brackets imply averaged over different microstates, you are taking a basically an ensemble average, right.

Now, how would you calculate these averages as the system accesses different microstates different spin configurations? Basically, the expression for the average energy here is summation over different microstates k . The energy of the microstate; so, after every month one Monte Carlo iteration everyone MCS: Monte Carlo Step, there will be a certain configuration of spins in the lattice which will correspond to a certain value of the energy E_i , right.

And the statistical physics formula is essentially the energy of a microstate into probability of accessing that microstate which is given by E to the power minus βE_i

by z , z being the partition function. This is the so called probability of accessing a particular microstate in a canonical ensemble, right.

But here in this in our case as we discussed we are doing a biased Monte Carlo simulation. So, what is a biased Monte Carlo simulation? We are basically accessing different microstates with the probability E to the power minus βE_i by z , right. Why that we will discuss it later. But with the algorithm which I discussed last time that already ensures that different microstates are being accessed with this probability. So, this is what I told you that met in the metropolis algorithm various microstates are accessed with probability e to the power minus $\beta \Delta_i$, it is a biased Monte Carlo all microstates are not equally accessed we are already using the background physics that we know to access different microstates.

Now, since different microstates with higher and higher energies are accessed with lower and lower probabilities, once a particular microstate has been accessed basically the average energy of the system is the sum of all the energies that the system accesses, all the different energies as the system goes on from one microstate to the other.

Sum up all the energies, and divided by the total number of Monte Carlo steps N MCS that the system remains in that particular thermodynamic state at that particular temperature, right. And you can control how many iterations you want to give for the system to remain in that temperature. So, in how many microstates you want to generate at a particular temperature, right and you can control that. And how would this is done and how this is chosen we shall discuss this later.

So, once you have calculated the thermodynamic quantities at a particular temperature what you can do is change the temperature, right. And allow the system to go to equilibrium, equilibria equilibrate at this new temperature, generate different microstates at a different temperature, calculate average energy magnetization C_v , χ , etcetera at that new temperature and keep on changing different temperatures, you keep on calculating this these quantities at different temperatures after suitable equilibrium. Then we what we do is try to do the physics, plot and monitor these various average quantities and how do they change with temperature and extract the physics out of it. So, this is the basic broad flowchart of what we shall be doing, all right.

(Refer Slide Time: 13:02)

The whiteboard contains the following text and diagrams:

QUESTIONS

- HOW DO WE KNOW HOW SYSTEM IS IN EQUILIBRIUM?
- HOW DO WE KNOW THAT THE THERMODYNAMIC AV. $\langle \dots \rangle$ IS GOOD ENOUGH AND RELIABLE?
- WHAT ABOUT FINITE SIZE EFFECTS?

spin (i,j)

BOUNDARY EFFECTS

SMALL SIZE OF LATTICE $\ll N_{AV}$

PBC (PERIODIC BOUNDARY CONDITIONS)

BUT

NEIGHBOUR OF $(L,3) \rightarrow (1,3)$
 $(2,L) \rightarrow (2,1)$

Diagram: A 3x3 grid of spins. The top row has spins $(1,1)$, $(1,2)$, $(1,3)$. The middle row has spins $(2,1)$, $(2,2)$, $(2,3)$. The bottom row has spins $(3,1)$, $(3,2)$, $(3,3)$. Arrows indicate interactions between adjacent spins. The grid is labeled with L on the top and left sides. Below the grid, the periodic boundary conditions are shown: $(i-1, j)$ and $(i, j-1)$ are connected to (i, j) and $(i+1, j)$ respectively.

Having discussed this immediately you should be having quite a few questions such as that how do we know that the system is in equilibrium. So, you have a lattice, you are generating different microstates as per your metropolis algorithm. When do we know that the system is in equilibrium? How do we know that the thermodynamic averages that we have calculated over a certain number of microstates, they are good and reliable? How do you know that you do not need to generate more number of microstates?

After all statistical physics tells you that basically the number of the ensemble average, I mean you have nearly an infinite number of microstates accessible. So, have you done a good thermodynamic averaging or not? Third question. What about finite size effects? After all we will be calculating or doing our simulations over a finite lattice, it might be 20 cross 20 or 100 cross 100 or 1000 cross 1000, if you are doing a 3D 100 cross 100 cross 100, lattice size is already 1 million lattice sites, you have 1 million spins it seems large for a computer.

Not for today's computer, but anyway it is a large lattice size. But what is 1 million spins? In statistical physics in a magnetic sample you essentially have 10^{23} spins setting on a lattice and you are basically interested to calculate the thermodynamic properties of a very large lattice, right. I mean why do you think that if you do your modeling and calculating of a thermodynamic averages over a even a 100 cross 100 lattice that is sufficient.

So, that is what is basically finite size effects. We shall be discussing each of these topics as we go along in the course, as we modulate in the computer I shall be showing how does one check for equilibrium, how does one check for whether the thermodynamic averages are reliable or not. So, all these will be discussed. But let us start with finite size effects.

Even within finite size effects there are two parts, I mean at least two parts, one could say that well there are boundary effects and the finite size of the lattice. So, we shall discuss this later. But let us talk about boundary effects. What do you mean by boundary effects? Well, you know you have in experimental in a real system you have 10^{23} atoms spins, magnetic moments sitting in even a small sample or if not 10^{21} which is anyway very large number.

And then at the end of the sample, right; so, if you have a material of this size say in the end of the sample basically those atoms are not surrounded by other atoms, but they are exposed to the air see, right. But the number of atoms which are setting on the surface of a sample of a macroscopic thermodynamic sample are relatively few, much smaller than the number of atoms which are in the bulk which is basically where atoms are surrounded by 4 atoms if you are talking of a 2D system or 6 atoms if you are talking about the 3D system, cubic lattice. Of course, you could also have triangular lattices, so we are not going into that at the moment but, assuming a square or a cubic lattice.

What basically I am saying that if you are doing a 100 cross 100 lattice or a 20 cross 20 lattice you have relatively large number of spins sitting at the boundaries and that number is relatively comparable to the number of atoms which are sitting in the bulk, the number of spins which have atoms spins which are basically surrounded by 4 neighbouring spins. Whereas, the ones on the right at the end these ones this, this, this there are they have only they have basically spins only on one side and not here, not here, right. And while we can neglect the effect due to the surface atoms on the in a real sample, can we really do it in this simulation? How do these show up?

So, the way we get rid of boundary effects in simulations is that we use periodic boundary conditions. What is periodic boundary conditions? You essentially say that you know what this atom, so this atom has one neighbour which is this one. So, the neighbour of this atom is this, this, this and this, right. So, now, so there is a continuity.

So, periodic boundary conditions you must have used also in your theoretical courses. Of course, this one has basically this neighbour, this neighbour, this neighbour and this neighbour, so it is not a problem at all. So, here this is how we get rid of boundary effects in simulations.

Now, let us say that this is spin i, j . So, suppose this is I am talking of this spin and this is basically spin i, j . So, that is how basically each site on the lattice is denoted by an array and choosing i and j basically fixes a particular lattice site. Now, one could say that the neighbour on the right can be denoted by the index the lattice index i plus 1, j . The neighbour on the left can be denoted by i minus 1, j , this being i, j ; this is being the spin of our interest.

The spin at the bottom, right; so, it is like one is can be denoted by i . While discussing this let me first set the convention I should have done this earlier. So, now, let us suppose that the spin on this corner is 1, 1, and then as you go on the right you are essentially increasing the index, so that this spin is called L 1, right. So, L, i plus 1, so this is 2, this is 3, whereas, the second index j remains the same, so this is L 1. Call this one essentially 1 L . So, basically y is increasing in this direction and this is L, L . So, in this convention basically the right neighbour of this one is i plus 1, that an left neighbour of this one is i minus 1, the down neighbour of this is i, j minus 1 and the one which would be here on the top would be j plus 1; i, j plus 1. Yes.

But you have a problem when you implement periodic boundary conditions because the neighbour of L 3, suppose this is L 3, right, so this is L 3. The neighbour of L 3 will be 1, 3. So, it is basically this one and the neighbour of 2, 1, right. So, what is 2, 1? It is basically this one, right; will be 2, L which is this one, right. So, when we calculate the neighbours and identify the neighbours we have to be aware and be careful about periodic boundary conditions. And this is how you identify neighbours. We shall see that in the code also later, ok.

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UNITS. MAGNETIC MOMENT $\vec{\mu} \Rightarrow \mu_B S_i$
 Bohr Magneton
 Spin $S \rightarrow$ angular momentum $\rightarrow \hbar \rightarrow \pm 1$.

MAGNETIZATION
 ORDER PARAMETER $\rightarrow \frac{\langle M \rangle}{M_{\text{max}}} \equiv \frac{\langle \sum S_i \rangle}{S_{\text{MAX}}} = \langle O \rangle$

AT LOW $T \rightarrow \langle O \rangle \equiv \langle M \rangle = 1$ (AT $T=0$)
 AT HIGH $T \rightarrow \langle M \rangle = 0$.

QUANTUM MECHANICAL CALC (eV).
 UNITS OF ENERGY $\langle E \rangle = \langle -J \sum_{i,j} S_i S_j \rangle$
 $H = -J \sum_{i,j} S_i S_j$ (IN SQUARE LATTICE).

So, the next thing to discuss before we actually move to the computer code and show how the algorithm is implemented is the issue of units. What do you mean by units? You already know that basically we are looking at magnetism, basically what is. So, we should be looking at the magnetic moment, but we know that the magnetic moment is essentially related by the Bohr Magneton to the spin of the system, right. And I am been telling you that the spin can either point up and down, and we will take its value to be plus 1 if it is pointing up and minus 1 if it is pointing down.

But, actually the spin of the system of an atom say is measured in units of angular momentum \hbar , right. So, when we say that the spin is plus 1 or minus 1 we are basically setting \hbar equal to 1, in after we calculate the magnetization we have to put back the units of spin which is a \hbar cross.

And, basically from the spin we can go to the magnetic moment by multiplying suitably by the Bohr Magneton. But all those are essentially set to basically we are ignoring that, we are saying yes the spin is just plus 1 or minus 1 instead of saying say minus half \hbar cross and plus half \hbar cross, right. So, that is all hidden for the purposes of the simulation. Of course, for the real system it is there.

Moreover, we are measuring magnetization when we use the word magnetization, we actually mean magnetic moment, which is the magnetization at a particular temperature. Well of course, having units of magnetic moment and we use magnetization as the order

parameter, but for purposes of the calculation we measure magnetization as the magnetic moment at a particular temperature which is essentially you know this angular brackets again represent the canonical ensemble average divided by the maximum magnetization possible which is can be only at 0 temperature, right. And this can be related to the average spin of the; so, average spin of the system at a particular temperature divided by the maximum spins maximum if. So, if all spins were basically pointing in the same direction say in the positive direction, so that would be the S MAX.

So, basically the number of spins on the lattice into plus 1 say and we use this normalized quantity as the order parameter to calculate the statistical physics, right. But of course, the units are there, though in the code we will not be really worried about the values of very small numbers like the Bohr Magneton and \hbar cross. Why? Because we can put it back in the calculation after we have finished our calculation and we do not want the computer to deal with very small numbers at as that will decrease the efficiency. So, you calculate it in so called simulation units and put it back when we want to compare with experiments.

Talking about order parameter, you already know that the maximum value of the order parameter. We have defined it in such a manner by suitably normalizing it that at low temperatures the order parameter is nearly equal to 1 or close to 1 and at exactly T equal to 0 it should be 1 which means the system is perfectly ordered there is no thermal fluctuations. Of course, there are quantum fluctuations, but we are at the moment treating the system classically which means that \hbar goes to 0, we are looking at only the thermal effects.

So, for classical spin system at T equal to 0, the order parameter magnetization will be equal to 1, which means it is perfectly ordered, all spins are pointing in the same direction and that is minimizing energy. Actually, I remind you and this is extremely important. In the thermodynamic system what is minimized is not the energy, but the free energy, but at T equal to 0 the free energy is $u - Ts$, T is equal to 0. So, energy minimization happens when all the spins are pointing in the same direction whether it be plus 1 or minus 1.

But any at any finite temperature the minima minimization of the free energy will be decided by $u - Ts$, the entropy of the system and the temperature as well and that is

why after all we get the phase transition. We will understand this better as we actually code it and we see the effects.

Anyway, because of the effects of entropy at high temperatures the what will matter in the minimization of free energy is not the contributions due to E , the average energy, the average internal energy, but rather the minus $T S$ term will dominate. It would rather the system will prefer to basically be in a disordered system, so that S is maximized through the minus $T S$ term, right. So, that is what it means. So, that dominates over the internal energy, right. The contribution of minus $T S$ dominates over the internal energy and that is how free energy is minimized.

Now, how to calculate average energy? So, we discussed order parameter here. Just to remind you we also, so we discussed order parameter magnetization, magnetic moment, the other quantity of interest is essentially the Hamiltonian, right, the energy. The energy comes from the expression for the Hamiltonian which is basically minus $J \sum_i \mathbf{S}_i \cdot \mathbf{S}_j$, where the summation is over although where i goes from 1 to N , N being the number of spins in the lattice $L \times L$ and the summation over the nearest neighbours J goes from 1, 2, 3, 4 in a square lattice, right.

And we also need to discuss what is going to be a units of energy. And what is energy? Essentially, energy is this average value of this quantity, of this quantity in the centre and this. So, this is basically the this quantity within the angular brackets is going to determine the spin of a particular of a particular micro state of or the spins are going to be arranged in a particular manner at the end of one Monte Carlo step. And that will depend the instantaneous energy of that lattice at the end of a microstate. And to calculate the thermodynamic or the average energy, right, one has to do this average over different microstates basically take an ensemble average.

You generate different microstates and calculate the energy, averaging over these microstates, right. Now we have to also discuss the units of energy.

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OTHER UNIT OF ENERGY IS $k_B T$.

$$k_B = \text{Boltzmann's Constant} = \frac{R}{N_A} = \frac{8.32 \text{ (SI units)}}{6.02 \times 10^{23}}$$

$$eV = 1.6 \times 10^{-19} \text{ Joules} \quad = 1.38 \times 10^{-23}$$

$$1 eV = \frac{1.6 \times 10^{-19}}{4.2 \times 10^{-21} (k_B T \text{ at ROOM TEMP})} \approx 0.38 \times 10^2$$

$$k_B T \text{ (at } T = 300 K) = 3 \times 1.4 \times 10^{-21} = 4.2 \times 10^{-21} \text{ Joules}$$

AT WHAT T VALUE IS $k_B T = 1.6 \times 10^{-19} J$ $\rightarrow \langle KE \text{ per particle} \rangle = \frac{3}{2} k_B T$

$$T = \frac{1.6 \times 10^{-19}}{1.38 \times 10^{-23}} = 1.16 \times 10^4 \approx 11,000 K$$

WE MEASURE $T (k_B T)$ IN UNITS OF J
 SET $J = 0.05 eV$ (SAY) $\rightarrow J = 1$.



Now, you know that this quantity J , so S_i and S_j you call it plus 1 and minus 1. And if you are saying that you want to calculate the average energy then the units of energy are essentially sitting inside this minus J . This is a minus J has all the Bohr Magneton, this, that everything. And so, J we shall be using as a parameter, but the value of J for different systems cobalt, nickel, iron, you can also get it using quantum mechanical calculations, right. And they typically J is measured in units of electron volts, so by doing the suitable quantum mechanical calculations, right, by putting in all the electrons all the various degrees of freedom, but here we are interested only in the magnetic moment degree of freedom.

The other unit of energy which is relevant in the problem is $k_B T$, thermal energy, right. It is basically a competition between as I said J which is determined by minus $J S_i \cdot S_j$ and the entropy of the system be where the spins can take different configurations minus $T S$. Now, how is $k_B T$ measured?

Now, k_B is the Boltzmann constant you might be knowing and that is written as R by N_A , where R is the gas constant $p v$ equal to $n r t$ that gas constant whose value is 8.32 in SI units. Whereas, N_A is the Avogadro number of atoms, k_B is R by N_A and Avogadro number of atoms as you might should be knowing by this now time is 6.02 into 10 to the power 23. And this gives the value if you divide it you gives 1.38 into 10 to the power minus 23 SI units.

$k_B T$, $k_B T$ has units of energy. You might have read in a statistical physics course, that using the equipartition theorem, the kinetic energy per particle mono atomic gas is $\frac{3}{2} k_B T$. Kinetic energy is essentially units of energy, so $k_B T$ has units of energy. And $k_B T$ at T equal to 300, T equal to 300 Kelvin which is essentially 27 degree centigrade is $\frac{3}{2} \times 1.4$, I have taken 1.38 to be 1.4×10^{-21} which is basically 4.2×10^{-21} Joules, ok. So, J is measured in electron volts typically and $k_B T$ is measured in say Joules. Now, we cannot be working with different units, so we have to set the units for our simulations, right and we want to have a easy unit.