Thermodynamics for Biological Systems:
Classical and Statistical Aspects
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Lecture – 85
Monte Carlo Simulations

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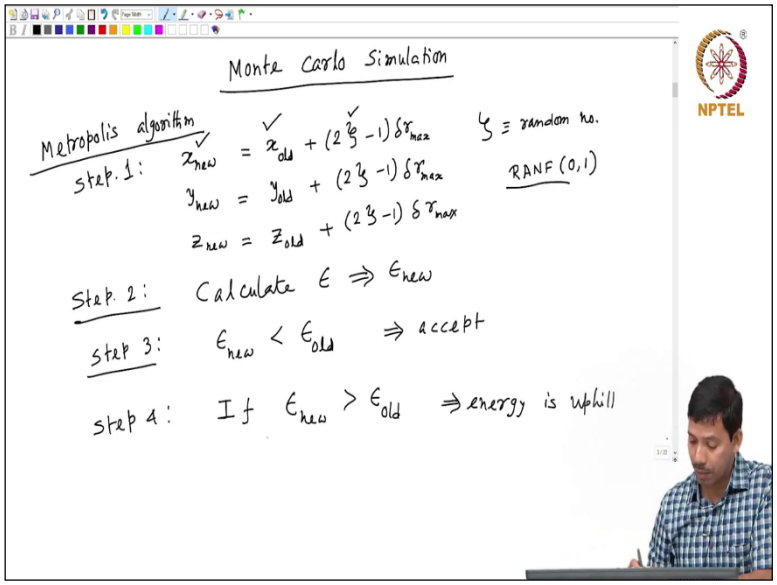

There is another computer simulation method which is called Monte Carlo simulation. We will go to the next slide which is called Monte Carlo simulation. So this is another simulation technique which is quite popular and this simulation method is also very useful to generate the different microstructures of your system.

So, I will briefly touch upon Monte Carlo simulation and here I will specifically look at the metropolis Monte Carlo algorithm metropolis algorithm which will guide us how to generate new confirmations, new micro structures of a system. So, in the metropolis algorithm there are four important steps so, metropolis algorithm, so, as I said that we are now trying to generate new confirmation of my system of interest, by Monte Carlo simulation technique.

So the metropolis algorithm is a very popular algorithm to generate any confirmation. So, in metropolis algorithm or in Monte Carlo simulations, the new confirmation of the system is generated by using random number generator. And that is the big difference of Monte Carlo with molecular dynamics. In molecular dynamics simulations we generated the new confirmations by solving Newton's equation of motion, Newton's second law.

We solved equation of motion to generate any of the confirmation whereas in Monte Carlo simulation we will be generating the new conformation of my system by using random number generator. So, in metropolis algorithm as I said there are important three steps. So, in step 1 what I will do is I will generate a new set of coordinates of my system randomly using random number generator.

So, if x_{new}, y_{new} and z_{new} are the new coordinates of ith particle I will generate I will obtain, x_{new}, y_{new} and z_{new} from my old confirmation. So, in in metropolis algorithm we will be generating the new coordinates of ith particle using random number generator. So, let us say x_{new}, y_{new} and z_{new} are the XYZ coordinates of my ith particle. And this x_{new}, y_{new} and z_{new} I will get as follows:
Step 1:

$$x_{new} = x_{old} + (2\zeta - 1)\delta r_{max}$$
$$y_{new} = y_{old} + (2\zeta - 1)\delta r_{max}$$
$$z_{new} = z_{old} + (2\zeta - 1)\delta r_{max}$$

Here ζ(zeta) is my random number.

And δr_{max} is the maximum displacement given to the particle. So, this random number you can use different functions available in a computer.

Usually there is a library called ranf random function RANF and this random number basically generate numbers between zero and one. So, with this random number generator, we will randomly create new set of coordinates, for my system and that will give me a new conformation. So, that was my step one. In step two I will calculate the potential energy of the system let us say my calculated potential energy of the system is U, in the new step I will calculate the new energy of the system.

And lets say that energy is E. The algorithm goes as follows:
Step 2:

$$Calculate\ \mathrm{E} \Rightarrow \mathrm{E}_{new}$$

step two is to calculate energy of the system and which is E_{new}.
Step 3:

$$E_{new} < E_{old} \Rightarrow accept$$

In step three I compared E_{new} with my energy in the previous step if E_{new} is less than E_{old}. If E_{new} which is a new conformation is having lesser energy than the older configuration then I accept this configuration or accept this microstructure.

Step 4:

$$If\ E_{new} > E_{old} \Rightarrow energy\ is\ uphill$$

In step four if my E_{new} is greater than E_{old} I accept it with certain probability. I do not discard it completely so this means my energy is uphill. When energies are uphill I accept this new configuration with the following probability.

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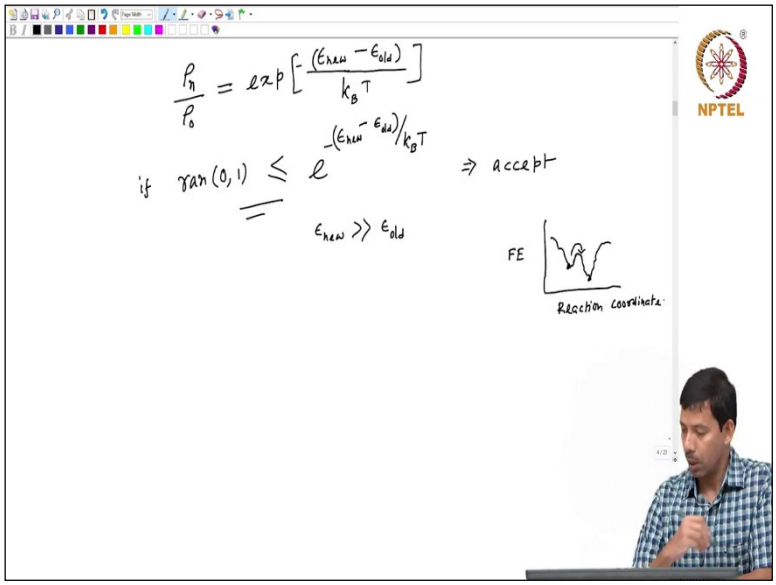

So, I calculate probability of the new and this is my old and I basically calculate the Boltzmann factor which is exponential minus E_{new} minus E_{old}. I calculate this Boltzmann factor. And if my random number so my random number is between zero to one, and then, I compare this Boltzmann factor e to the power minus E_{new} minus E_{old} divided by KBT. I compare with this.

$$\frac{\rho_n}{\rho_o} = \exp[-\frac{E_{new} - E_{old}}{k_B T}]$$

$$\text{if ran}\,(0,1) \leq e^{-(E_{new}-E_{old})/k_B T} \Rightarrow accept$$

If this is valid I accept this why I accept if this condition is fulfilled, so, this is valid only when my E_{new} is not too big. If E_{new} is just little bigger than E_{old}, then, what will happen? So, this difference is close to zero and then this whole Boltzmann factor is one so this is fulfilled that

because one is more than any number between zero to one, so I accept it. If my E_{new} is very large than E_{old} then this Boltzmann factor becomes close to zero and this condition does not fulfil.

$$E_{new} \gg E_{old} \implies reject$$

So I do not want to get our configuration which is having a much higher energy, than the previous configuration, because I am having a very higher energy configuration and I do not know whether that is good configuration or not. On the other hand, if I generate a configuration which is having energy just little more than my previous configuration, I tend to take that so that, you know I always may not go in my energy profile below.

I might have small energy barrier and then I might go to a better energy state. So, I should not just get trapped in this local minima I should take up some configuration which will allow me to cross this barrier and can get to a better conformation. So, this is my free energy profile with reaction coordinate okay. So, thus the Monte Carlo simulation, here one thing I need to stress is that, when I, when I am generating the new conformation I am trusting or I am using only the preceding state.

I am generating new configuration only based on my preceding configuration. I do not care what was the configuration before x old? And that is where Monte Carlo and molecular dynamics differ.

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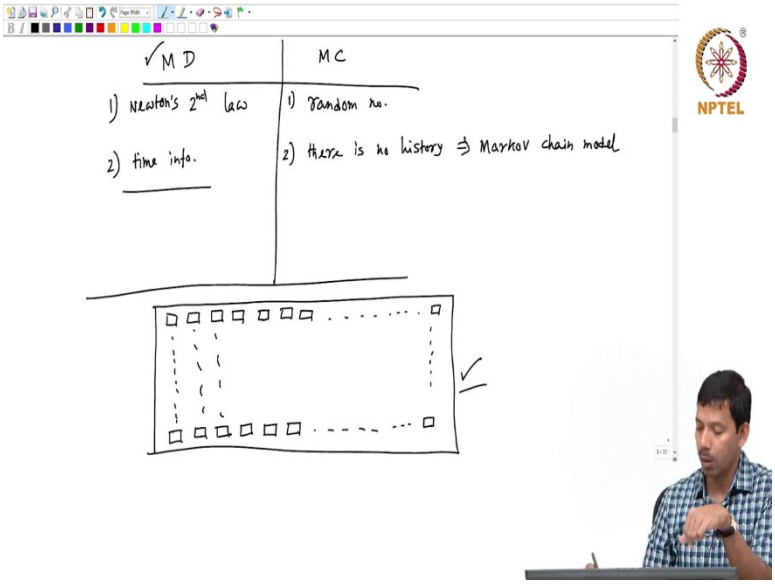

So, if I compare molecular dynamics and Monte Carlo. So, first difference the most important differences in MD, we basically look at Newton's equation of motion. We solve Newton's second

law by solving equation of motion whereas in Montecarlo we generate the new configuration by random number. So, we use the random number generator to generate the configuration randomly.

And the second difference between MD and MC is that here there is a time information because we are solving force is equal to mass into acceleration and acceleration has the time information and therefore there is a time information present in MD where as in Monte Carlo simulation our new configuration is depending only on the preceding step and it, it does not have any memory, about what was the configuration before the preceding state.

And that is called the Markov chain model. Also in Monte Carlo there is no history and that it follows a Markov chain model. Nevertheless both the MD and MC simulation techniques help you which I am emphasizing again is that these techniques basically help you to generate your ensemble it basically helps you to get all possible microstates of your system, so that you can, calculate the thermodynamic properties in the accurate level which matches the experimental data.

So, both MD and MC are generating a lot many microstates and when you put up this information of the microstates, you see the time evolution when you are talking about MD, there is no time evolution from MC but ultimately when you take the average of the ensemble you get the property which you can compare with experimentally measured property which are the macrostates.