Thermodynamics for Biological Systems:
Classical and Statistical Aspects
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Lecture – 84
Calculation of LJ Force

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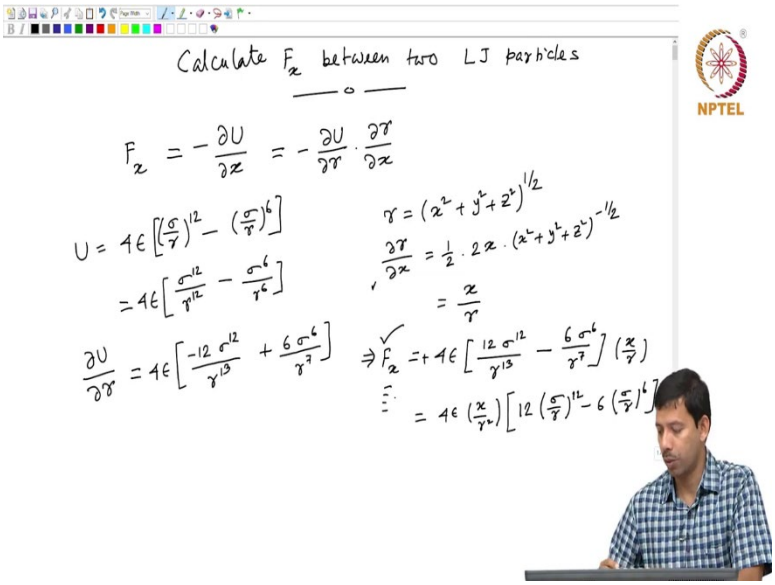

Now let us calculate Fx the x component of force between two Lennard Jones particles so, what we are trying to do is calculate Fx, x component of force between two Lennard Jones particles. This is a very similar problem of what you did previously, what you wanted to calculate effects between two ionic particles, which we said the Coulomb particles. So, here when I say 2 Lennard Jones particles that means the particles they follow the Lennard Jones potential when they interact with each other.

So, when you want to calculate the Fx essentially what you have to calculate is gradient of potential with respect to the x component.

$$F_x = -\frac{\partial U}{\partial x} = -\frac{\partial U}{\partial r}\cdot\frac{\partial r}{\partial x}$$

Now, my U as the question said is described by Leonard Jones potential so my U between two particles could be

$$U = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

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So, from here you want to calculate $\frac{\partial U}{\partial r}$. If you differentiate U with respect to r what you will get

$$\frac{\partial U}{\partial r} = 4\varepsilon \left[\frac{-12\,\sigma^{12}}{r^{13}} + \frac{6\sigma^{6}}{r^{7}}\right]$$

That is your derivative. And what is $\frac{\partial r}{\partial x}$.

$$r = (x^2 + y^2 + z^2)^{1/2}$$

$$\frac{\partial r}{\partial x} = \frac{1}{2} \cdot 2x \cdot (x^2 + y^2 + z^2)^{-1/2}$$

$$\frac{\partial r}{\partial x} = \frac{x}{r}$$

Simple substitution leads your x component of force

$$F_x = +4\varepsilon \left[\frac{12\sigma^{12}}{r^{13}} - \frac{6\sigma^{6}}{r^{7}}\right] \left(\frac{x}{r}\right)$$

$$F_x = \left(\frac{x}{r^2}\right) \left[12 \left(\frac{\sigma}{r}\right)^{12} - 6 \left(\frac{\sigma}{r}\right)^{6}\right]$$

So that is your x component of force between 2 Lennard Jones particles. Likewise you can calculate the force between two interacting particles along the Y direction along the Z direction and so on.

So now the question is what is the relevance, what is the relevance of calculating the x component of force between the Lennard Jones particles or between the Coulomb particles.

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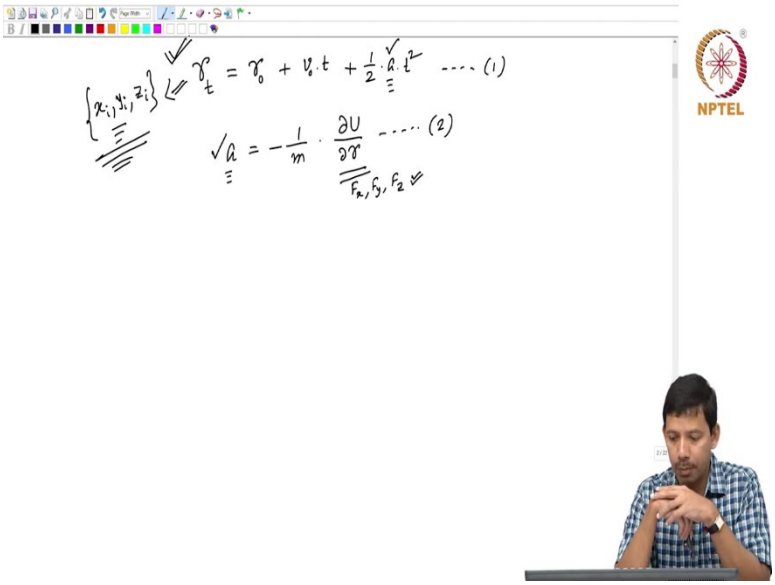

That is because if you recall how we propagate our system in molecular dynamics is that we make use of two important equations expressions. And those are

$$r_t = r_0 + v_0.t + \frac{1}{2}.a.t^2 \qquad eqn\ (1)$$

this was equation number 1 and we have the other expression

$$a = -\frac{1}{m}.\frac{\partial U}{\partial r} \qquad eqn\ (2)$$

a is equal to minus 1 by m del u del r. That is my equation number 2. So, these two are the primary equations in my molecular dynamics simulations. Our ultimate goal is to get r (t) which is nothing but a set of x y and z i coordinates and that they basically define the location of each atom in your system and when you put up all these atoms together then you see your whole system.

So our ultimate goal is to get X Y Z coordinates for each of the ith particle and for that we need to get the X Y Z components of a. And to get that XYZ component of a, you need to calculate force along X Y or Z direction. So, you need to calculate these force components during your calculations. And those will give you the acceleration and that when you feed in equation number 1, you get this new set of coordinates, which give you a new microstate or a new confirmation of your biomolecule of interest.

So, there was the relevance of calculating the force component okay. So, the next thing what we will be looking at is, is something where we can calculate different microstates of a system by another computer simulation method. So, if you recall why we introduced MD in our discussion

is that we know that ensemble is comprised of lot many microstates and so those microstates are basically giving the microstructure of our system.

And to generate the microstructure in a large number for my system of interest, we introduced molecular dynamics simulation. And this technique basically given us the clue how to generate different new confirmations or different new microstructure of my system of interest.