Thermodynamics for Biological Systems:
Classical and Statistical Aspects

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Lecture – 72
Computer Code for LJ Potential

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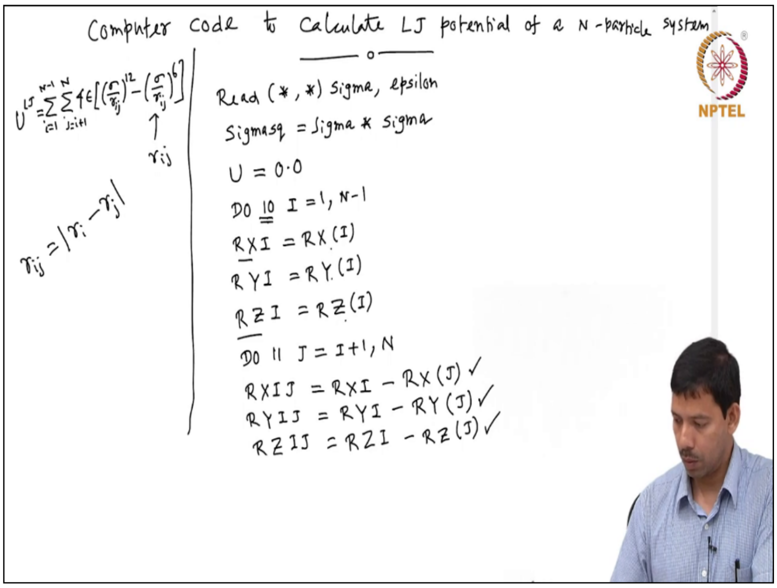

Let us write a computer code or what will be the logic of a computer code to calculate the Lennard-Jones potential for a system of n particle system. So, what I am basically trying to do now writing a computer code to calculate Lennard Jones potential of our N particle system let u try writing out a computer code and writing this is in Fortran 77 you can; so, basically I will be presenting the logic and then you can write in your own language of C C++, fortan 90 and so on.

$$U^{LJ} = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right]$$

$$r_{ij} = \left| r_i - r_j \right|$$

So, this is a computer code what I will be writing in Fortran 77. So, we have n particle systems and we want to find out the Lennard-Jones potential. So, if you recall the Lennard-Jones potential it was okay so my Lennard-Jones potential was ULJ is equal to sum over i sum over j for Epsilon Sigma by r ij to the power 12 -Sigma by r to the power 6. So, this is the this is a formula what you will be executing so as I said that for the pair potential to have had the same interaction twice we put in equality where my i goes from 1 to n - 1 and jfrom i + 1 to n.

If you put this if you maintain this limit then you are not over counting the same interactions you are not counting the same interaction twice you are not counting to 1 since you already have counted one two interactions ok. So, to do this first we have to know the value of epsilon and Sigma epsilon and Sigma there the constant values so they do not change. So, what is the variable here we have is basically the r ij and what is r ij? r ij is nothing but your ri - rj sorry it is the inter particle distance the distance between particle i and j.

$$Read\ (**) sigma, epsilon$$
$$Sigmasq = sigma * sigma$$
$$U = 0.0$$
$$DO\ 10\ I = 1, N - 1$$
$$RXI = RX(I)$$
$$RYI = RY(I)$$
$$RZI = RZ(I)$$
$$DO\ 11\ J = I + 1, N$$
$$RXIJ = RXI - RX(J)$$
$$RYIJ = RYI - RY(J)$$
$$RZIJ = RZI - RZ(J)$$

And that is a only variable so that you have to calculate inside the loops and epsilon and Sigma are the constant values which you can read directly. So, we will start by reading epsilon and Sigma. So read I can leave this on the screen itself and read Sigma and Epsilon. And after I read that I am calculating Sigma square. So, Sigma square I am calculating by multiplying Sigma with Sigma. So, this is my Sigma square.

Now i initialize my potential by setting it to 0 so I am now initiating the calculations. So, my U to start with is 0, now I start my to look Do i is equal to 1 to N - 1 and my RX I is equal to RX I my R YI re so basically I am reading the X Y and Z coordinates of each particle. So, this is the X coordinate Y coordinate Z coordinate of the particle same reading 1 to n - 1 particles X Y and Z coordinates. Now since I have to calculate the pair interactions.

Interaction of I with j inside this two loop I have another Do loop which is j ok so I have to give some number let us say I am sorry so in the; here I need to put number, so Do J so this is Fortran do J root N I is equal to 1to N - 1 so this is my anti loop with you know 10 is basically number which I started here and I need to close it later. So, I start on the loop do 11 J, so J goes from I + 1 to N. So, now inside this I now calculate RX IJ so which is basically the distance between the X component of Ith and Jth the particle.

So, I already have our X I from here so I write RX I- R XJ, so this is my X component separation between ith and jth particle. Similarly RY IJ, I can write as R Y I- R Y J R Z IJ is equal to R ZI which I already have minus R Z Jth particle. So, here basically I am looking at the separation of X coordinates of I and J separation of the Y component of I and J and the Z coordinates of I and J.

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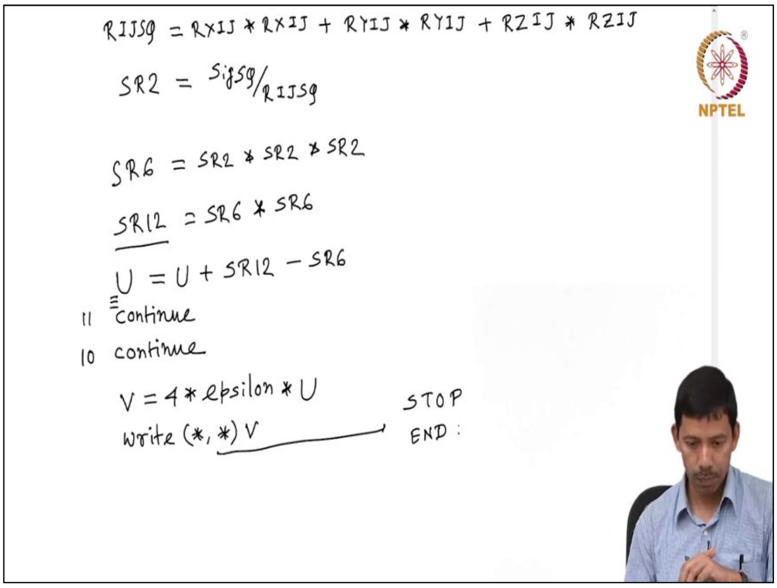

$$RIJSQ = RXIJ * RXIJ + RYIJ * RYIJ + RZIJ * RZIJ$$

$$SR2 = \frac{Sigmasq}{RIJSQ}$$

$$SR6 = SR2 * SR2 * SR2$$

$$SR12 = SR6 * SR6$$

$$U = U + SR12 - SR6$$

$$11\ continue$$

$$10\ continue$$

$$V = 4 * epsilon * U$$

$$write\ (*,*)V \ldots\ldots\ldots\ldots..stop\ END$$

Then what I have to calculate is the R IJ square because the distance between two particles is square root of X I - XJ square + Y I - YJ square + ZI - ZJ square. So, RJ square since I already have RX IJ and R so I have RX IJ RY IJ RIJ so RX IJ multiplied by RX IJ + RY IJ plus so this is my R IJ square and what I need is 12 and 6 so from here I can define a SR2 so easily this very short range. So, Sigma square because Sigma square divided by RIJ square likewise I can define us R6 which is SR2 multiplied by SR2 multiplied by SR2.

And SR12 is nothing but it is SR6 multiplied by SR6, so my SR12 is nothing but Sigma divided by R to the power 12 and SR6 is nothing but Sigma by R to the power 6. So, now I need to sum them up so my U is instantaneous value of U plus SR12 - SR 6 and now I need to close my Do loops so that Jth loop is an inner loop so I need to close that first and then I close the outer loop after I closed the Jth loop.

And once the loop both loop are closed I get that total U which should be multiplied by 4 epsilon I have read and this 4 epsilon the constant term I have to multiply with the U the final U I get after the loops are closed so this would be mine final out potential Lennard -Zones potential so which I can write on the screen as V and then I can then I have to basically say stop at end so from here I have two more steps stop and then end that will be my Fortran 77 code to calculate Lennard Jones potential of N particle system.