Thermodynamics for Biological Systems:
Classical and Statistical Aspects
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Lecture – 80
Idea of Z-Matrix

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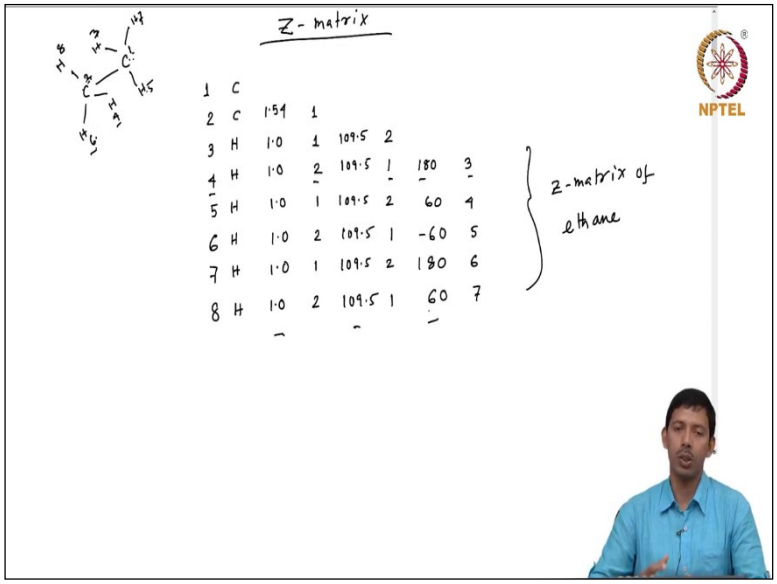

Now what is the Z matrix?

Z matrix as I said, it basically writes internal coordinates of a molecule in a more tractable form? So, let us say I am taking the example of ethane. So in ethane I have carbon I have another carbon and I have CH3 here and a CH3 here. I just named them as 1 atom 2 atom 3 atom 4 5 6 7 and 8. So, to write the Z matrix first I write my number 1 atom is carbon here, number 1 is carbon number 2 is also carbon, so now number 2 atom is connected to number 1 atom.

So 2 is connected to number 1 atom by a bond distance of 1.54 Angstroms this is in Angstroms. Now what is my atom 3, my atom 3 is hydrogen and that is connected to 1 by a bond distance of 1.0 angstrom 3 is also making an angle with 3 1 2 so I write your 3 1 2 and the angle is 109.5 number 4 atom is a hydrogen which is bonded to 2 by a distance of 1 and it makes an angle of 4 2 1 again, so I had angle 4 2 1with the same angle of 109.5.

Now this also makes a dihedral so my angle is 4 2 1 3, so I can write 4 2 1 3 so that is a dihedral and that dihedral value is 180 because this is a staggered conformation of ethane. So, here you can see that 4 2 1 3 forms a dihedral of 180 degree. Similarly 5 is also hydrogen connected to 1

by 1.0 it makes an angle of 5 1 2 of angle value 109.5 it forms a dihedral with 5 1 2 4 and that angle is 60 degree.

Six forms, so it is also hydrogen atom forms a bond with 2 of bond distance 1, 6 forms angle with 6 2 1, angle is again 109.5 degree and 6 forms a dihedral with 6 2 1 5, forms a dihedral of – 60. I just erase that – 60. Number 7 is hydrogen forming a bond with one and that value is 1.0 and the angle it makes with 7 7 1 2 again 109.5. So, now atom number 6 is also a hydrogen which forms a bond with 2 of 1.0, 6 forms the angle of 621 with a value of 109.5 and then it also form dihedral 6215 and that dihedral angle is -60.

Atom number 7 which is a hydrogen forms a bond with 1 of value 1.0, 712 forms angle of 109.5 and 7124 or 7126 we are trying to cover all possible the dihedral angles and that is 180 so that the full structure of the molecule is defined. Number 8 is a hydrogen connected to 2 by a bond distance of 1.0, 8 2 1 angle and angle of 109.5 and with 8 2 where is my 8, 8217 here is my dihedral of 60 degree okay. So, this is the Z matrix of ethane.

So if I have Z matrix then I can easily get the bond angle and the dihedral quickly instead of looking at the XYZ coordinates of each atom and calculate bond angles and dihedral to make my calculations faster. So far what we have seen is that we can have our initial coordinates from protein data bank or if there is no structure available we can generate a crude structure from homology modelling if you are interested for a biomolecule or you can make a simple model by drawing by chemdraw if your molecule is small and then you choose the right force field parameters.

So, choosing the right force field parameters is important because some scientists are interested in water soluble proteins so there force field parameters will be different than our set of parameters which are made with the aim of covering the membrane proteins for example. Since membrane proteins are less water soluble versus the other set of proteins which are cytosolic proteins.

So the parameter is developed in these window versus that window will differ. So, if you choose force field parameters which are made for membrane proteins and now you are picking up those parameter files for a cytosolic protein and running simulation, your results will not be very good.

So, that is another conceptual understanding you should have when you want to generate the different microstates of your system of interest.

So you got the initial coordinates you chose the right force field parameters and then you now know the different tricks of the MD simulations, the technique by which you will generate different microstates and by those tricks you made your simulation much more practical in a sense that you are giving your protein or your liquid a bulk like behaviour so that there is no surface effect so surface effect will be dealt with periodic boundary condition.

Then you have that minimum image convention to cut down the number of original interactions to the same half of n into n -1. And then you used another trick called cutoff by which you further cut down the number of interactions to make your calculations faster. So, you are ready to generate the new confirmations or the new microstates. So, how do we do that? So now we will talk about how we propagate our system how do we generate new microstates starting from a given microstate.

So my given microstate is basically the initial coordinates which basically put up together which will give you an initial structure.