Computational Chemistry & Classical Molecular Dynamics
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Lecture – 38
Molecular Dynamics using Gromacs-6: Mixture of Water and Methanol

Hello. We will continue our discussions of gromacs simulations. So last time we did the simulation for water. We did the distribution functions as well as the diffusion constant. Now we want to extend this approach to mixture of 2 solvents. In this case, what we are taking? Water and methanol.

So all this discussion is for a, this mixture and we will continue with this discussion. Okay start with the file structure now. Yes, so to perform molecular dynamics simulation of water-methanol mixture, we need, first of all we need the pdb file or the structure file for water.

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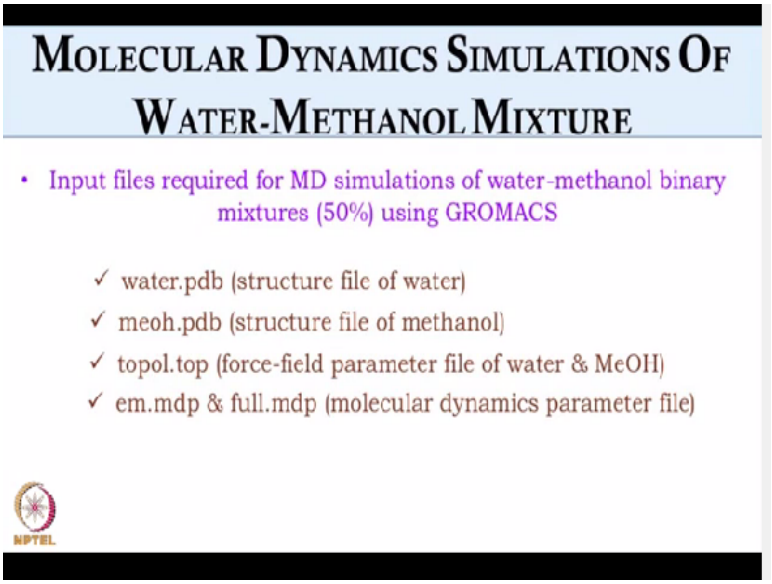

We will also need the structure file of methanol which is meoh.pdb. Then we will need the topology file for, which will contain the force field parameter of water as well as methanol and we will need molecular dynamics parameter file, that is the mdp file for energy minimization as well as for molecular dynamics simulation. Yes, so before we proceed, we have to first decide what composition we want. Yes. So we have chosen a 50:50. 50%. Okay.

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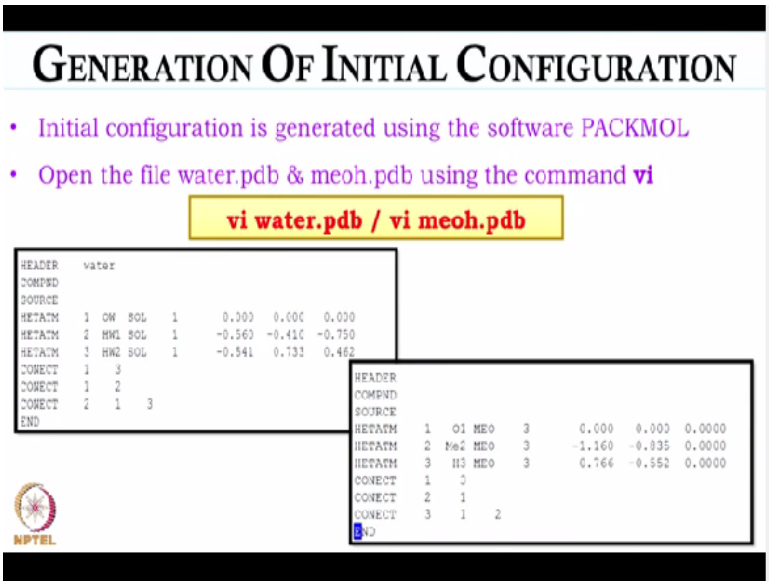

Here also the initial configuration is generated using the software PACKMOL. So just open the file water.pdb and meoh.pdb using the command vi. So vi water.pdb and vi meoh.pdb. So water structure, I have already discussion earlier that water, like the last 3 column represents the coordinates of oxygen hydrogen and 2 hydrogen in x y z axis. Then sol is a residue name. Then there is bond connectivity and angle connectivity.

And this is the pdb file for methanol where we have taken methyl group as united atom. Like we have taken methyl as one group and then there is oxygen and hydrogen. So and the residue name of methanol is meo and this is the coordinate of x y z axis and connect 1 3 and 2 1 which means that the bonds are connected, like O1 is connected to methyl and O1 is connected to hydrogen. And connect 3 1 2 is the angle connectivity.

So now those on the extreme right are the coordinates of oxygen. Methyl. Of methyl group. And hydrogen. And hydrogen. Yes. Again in angstrom units. Again, yes. It is in angstrom, since it is a pdb file. So 1and 3 are connected and. 2 and 1 are connected. So instead of 2 and 1, can I give 1 and 2. But, just a sec, 1 and 3? Yes. And you want to give 2 and? 1 and 2. Yes, 1 and 2 is fine, because anyways O and H and H and O connected. Okay.

So given as well give 2 and. Instead of 1 3, I can give 3 1. Yes, not an issue. And instead of 3 1 2, can I give 2 1 3? Yes, you can give 2 1 3. Okay. CH3OH, yes, I think can give as well. Okay. And

again the bond angle can be calculated using vectors? Yes. And bond length can be calculated just by distance between 2 sites? 2 sites, yes. Okay. So now since we have pdb files, so we have to specify what numbers we are going to take and what is the box length we are going to take in inp file which is the input file in PACKMOL.

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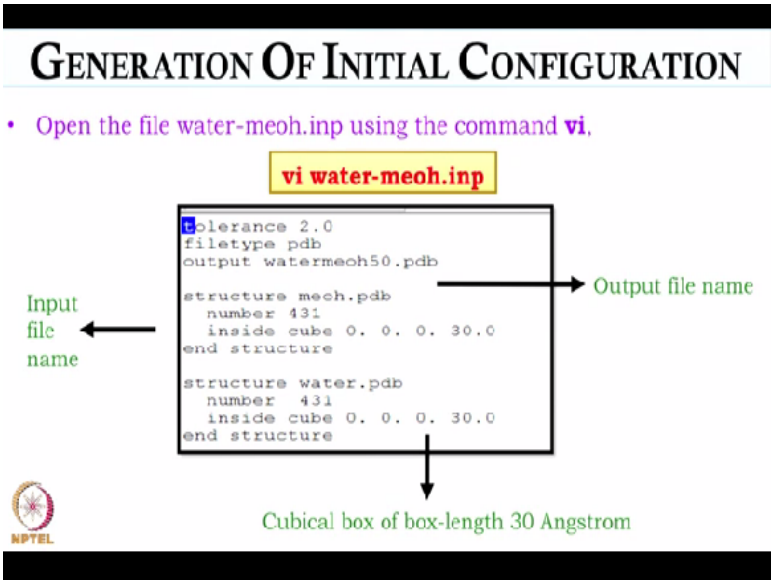

So this is the, the inp file name is water-meoh.inp. So if one wants to download an inp file or wants to see what an inp file for a mixture looks like, one can go to the site packmol and there they will have water-urea inp file which is the binary mixture of water and urea. In an input example, they will have the file. They can download the inp file. They can download the pdb file of water and urea as well.

But can we not take the inp file for the 2? Yes. And create for the mixture? It is the same thing actually. So I will just show you the inp file. Okay. So this is the inp file for water-methanol mixture. Okay. Whatever we have taken in case of water, right, we have taken water, structure, number inside cube and end structure, we just have to repeat these 4 lines for methanol also. Because methanol is also being added to the mixture, so we just have to add these 4 lines for methanol.

You change the name of the output file. You just have to add structure meoh.pdb which is the pdb file of methanol. You have to specify the number, what is the number that you are going to take.

And the box length. Can the order be changed? Yes, the order can be changed. Instead of meoh.pdb first and those lines? Yes, yes, the order can be changed. So order can be changed. Okay.

Not an issue. So then... Then why have you called it water-meoh50.pdb? Because this is the water-methanol mixture. 50%. And 50% mixture. So to get a, to have a clear idea. Suppose you are doing more and more simulations, so you have many output files. So you will have a clarity. So it is good to have a file name which reflects the final composition or the initial composition. So that you do not get confused.

So this is the output file name watermeoh50.pdb and 30 is the cubical box of box length 30 angstrom. So it is designated inside cube. Okay. So now we will execute packmol using this inp file.

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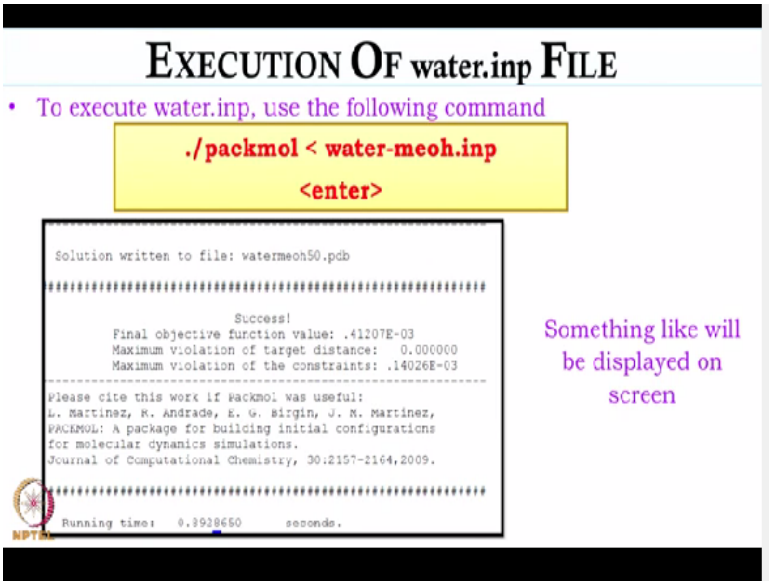

And we will use the same command, ./packmol<water-meoh.inp. So after the successful execution, we will have something like this displayed on your screen, like solution is written to file watermeoh.pdb and then what is the time it has taken to complete it. So now we have the pdb file.

So now we will create mixture.pdb, mixture directory or mixture50 or watermethanolmixture

directory in the working directory. Gromacs directory. Yes, in the gromacs directory and then we will copy the file watermeoh50.pdb to that directory so that we can convert it into a gro file and we can proceed towards the simulation. Okay.

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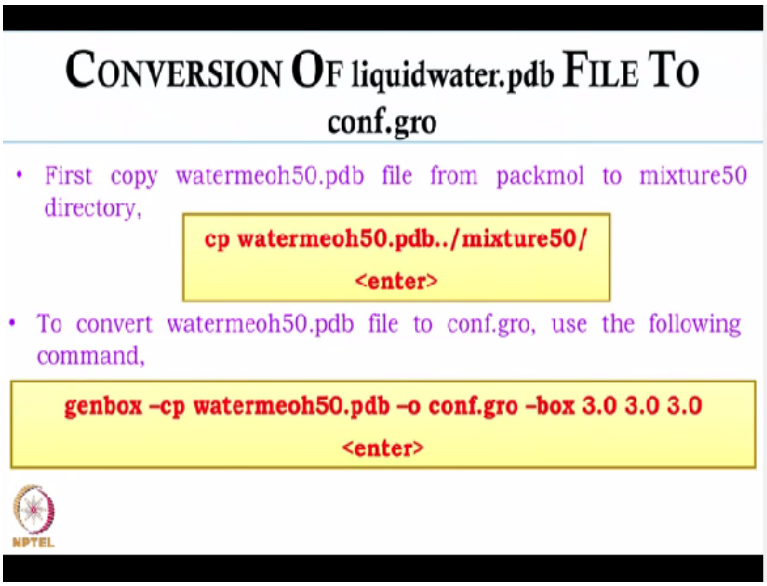

So now we will convert the liquidwater.pdb file, sorry watermethanol50.pdb file to conf.gro file. Okay. So we will first copy this file. So to copy, we will have to type the command cp. So you have must already make directory mixture50. mixture50, yes. And then copy to that directory. Yes. Again there should be space between the 2 dots? Yes. Okay. So now the file will be copied and now to convert this pdb file into a gro file, we will use the command genbox.

So genbox -cp, which is a flat for input file watermethanol50.pdb, then space -o which is for output, space conf.gro which is my output file, then space -box. -box and after that we have to give the bond length. The box length. The box length in nanometer which is 3 3 3, it is a cubical box of 3 nanometer. And then we type enter.

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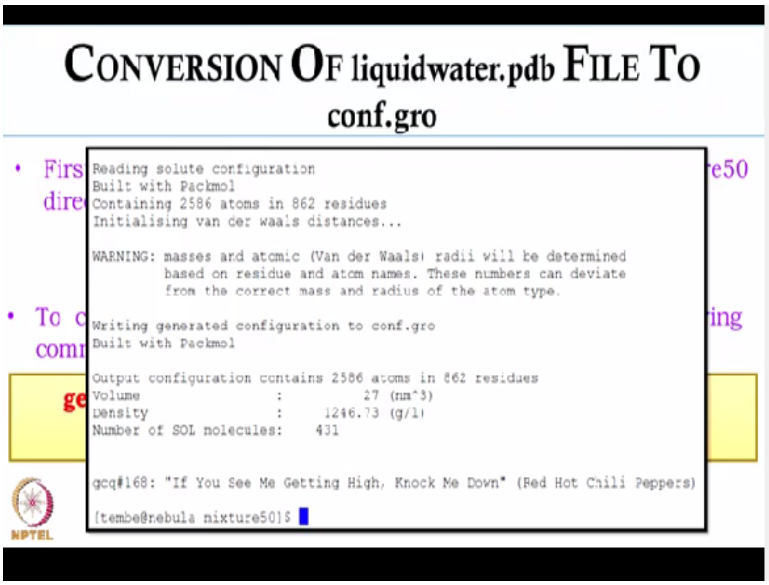

And after that something like this will be displayed. So it will read the solute configuration which is built with packmol. So there are total 2586 atoms and 862 residues because there is 431 water and 431 methanol molecules. So total 862. And then it will show the volume, density, number of solvent molecules. So this density is the total density? Total density of the mixture. Okay that is the volume.

So it is saying number of solvent molecules 431? Yes. Now suppose you did not have a 50:50. Yes. Then will it show 2 numbers there? Yes, it will show 2 numbers there. Or it will show one of them because the... Other one is self understood that what will be. Total, right. Other one, yes. So now that there are 862 molecules, this was not predetermined? Yes, this was predetermined. Because you will have a density of water-methanol mixture.

Okay. Right, you know the density of water is 50% mixture density. From that density you calculate the number of molecules for water and for methanol. So that 1? 246.73. What is the unit there? g/l. Okay. So this density you got it from experimental density? Yes, this is the experimental density. Of the mixture? Yes. Okay. But one thing I want to tell all the (()) (08:38) is that when we calculate these densities, does it worry about the partial molar volume and things like that or it just numerical calculation?

When we calculate the number of molecules? Right. Because see when you mix water and

methanol. Yes. The total volume is not the sum of volumes. No. Right. So this is really other complex issues. So what we do in simulation, we just take the total number. Yes. And do not worry about partial molar volume. For the initial calculation. Yes. But if you want to do those calculations, there are ways of doing it later on.

Yes. So we will just find the total density and mix them in proportions. Yes. And make sure that it is closed to experimental density and proceed. Yes. Okay. So although there were separate pdb files, now there is only 1 gro. 1 gro file which will contain. Information of both. The way you have given in packmol the inp file, suppose in inp file, first there is methanol pdb and then there is water pdb.

So in gro file, you will have first methanol. Right. Coordinates 431 and then you will have water coordinates 431. Okay. So the sequence you have given packmol's inp file will be reflected in the gro file. It will have the same sequence. So now we have to go to the top file. Yes, now we will have. Will there be 2 top files or 1 top file? 1 top file but there will be 2 itp files. Why is that?

Because water and methanol molecules are different. In top file, you just have to write sigma epsilon and charge. So you write for all of them? You can write for all of them. First you can write for methanol and then you have to write for water. Because you have to maintain the same sequence throughout. Okay. Right.

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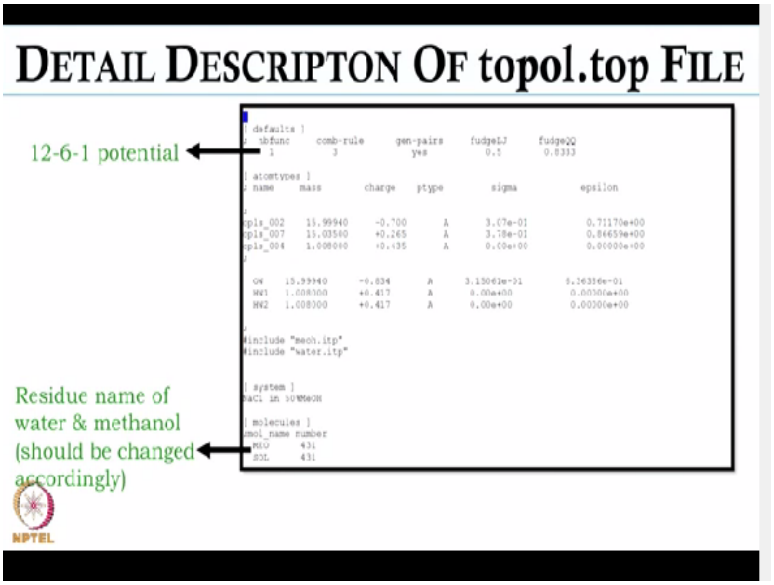

So now I will go to the top file. So this is the top file, right. So npfunction is the nonbonded function, 12-6-1 potential. Combination rule 3, I have already saved earlier. So here you see that first there is opls_002, then 007, then 004. This is for methanol. Since for methanol we are taking opls force field. So the first one is for methanol and opls_002 is for oxygen. So the mass is given there.

Then 007 is for methyl group. Since you are taking united atoms. And then opls_004 is hydrogen atom. So in your second column are the masses, the third column is the charge? Yes. And what is that ptype A A A? (FL) So this is... Just move it a little, yes. Yes. So this is charge. This is charge on oxygen atom. This is on methyl group. Okay. And this is on hydrogen atom. This is, ptype is, this is atom type.

Okay. A is for atom. Okay. Then this is sigma in nanometer and this is epsilon in kilojoules/mole and this is for water molecule. Okay. This is oxygen and 2 hydrogen. Okay. So this is the mass of oxygen and hydrogen. This is the charge is on each of the atom. This is again atom type and this is sigma and epsilon values. So that whatever opls_002. Yes. It is given by the system or? No, no, no.

You have to include it. Because see you have to have the charge of oxygen methyl group and hydrogen atom, right. You have to get it from somewhere. You cannot put some random values

of sigma and epsilon. So what do you do is? You go to the top folder which you will get when you install gromacs. Right. And then inside the top folder, you will have opls folder. Okay. Right.

So you got the first 3 lines for methanol from the opls folder? Yes, from opls, you will have ffnonbonded.itp and then there you have to go, search for methanol oxygen atom charge and oxygen atom, methyl group's charge and hydrogen atom's charge. And from there you will get sigma and epsilon values. Okay. And then you have to include itp file for methanol and water. So this, here also you have to maintain the same sequence.

First you have to write for methanol and then you have to write for water. So for the ptype, you have given A A A. Yes. Can you give B B B? No it is only A type allowed and if you give residue, then you have to write R. R only. Yes. Okay, so either it is A or an R there. Yes. Okay, then? And then you have to include the itp file for methanol first since in pdb file, we have methanol first and then water.

So methanol first and then water and then you have to define your system. You can write anything in there. And then you have to write, molecules you have to define. First is meo. No, no before we do that, after the 2 includes, you have 2 blank lines. We will give those blank lines? You cannot give the, you do not require the blank line as well.

But just to get a clear picture. So after the system. Yes. There is something NaCl, what is that? That is to define the system. You can write anything. You can write 50% water methanol mixture, anything you can write, it does not count. Okay that is just a; to define a system, you are just defining your system. Okay.

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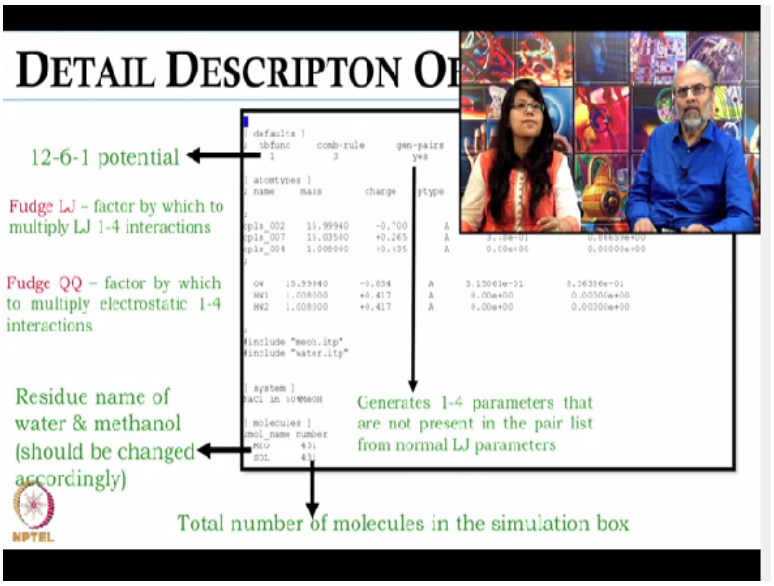

And then you will have molecules type. Right. So here you will have to give the residue name of the molecule. So since we have meo in the first, so we will have meo as the residue name. Okay. Then the total number that is 431 and then sol, that is solvent that is 431. Right, right, okay. So this is the topology file, right. So this I have already told that it will generate 1-4 interaction and then fudgeLJ and fudgeQQ are for LJ 1-4 interactions and for electrostatic interactions. Okay.

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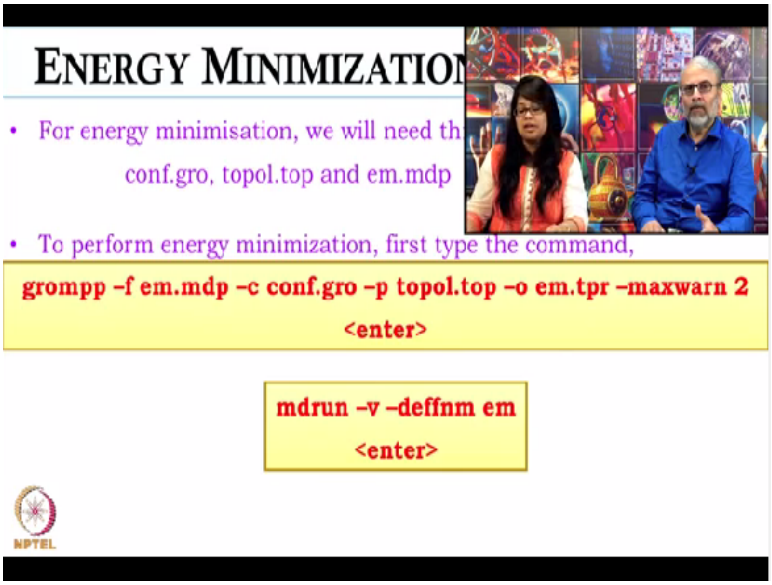

And now we will proceed, now since we have gro file, we have topology file, so you will proceed towards the energy minimization of the mixture. We will use the same command and we will use the same em.mdp file. So we will first generate the tpr file using the command grompp. So we will combine mdp. So from now onwards, there will be only 1 file now, not 2 because we

have already combined everything.

Yes. Into 1 file. Okay. So we will use the tpr file, because in em.mdp file is same. Okay. In conf.gro, we have all methanol and water molecules coordinate. In topol.top, I have already included water and methanol's itp file and it already contains information like sigma, epsilon, charge of both water and methanol molecules. So I do not have to include different file for water and methanol.

Okay. And now I will generate em.tpr file which will be my input for mdrun for energy minimization. So I will just type the command mdrun -v -deffnm em which will generate all my file, output file which will have initial as em. So now what we are doing, calling everything by em? Yes. So which means in each directory, there will be several em files? Yes. Okay.

So it is very important to keep the directory structure intact? Yes. Because if any mistake is there, everything will be gone. Yes, yes, yes. Because we are performing in separate directories, right. So in water, we will have water "ka" em. In mixture, we will have mixture's em. Okay. So directories have to be different. Okay. Right.

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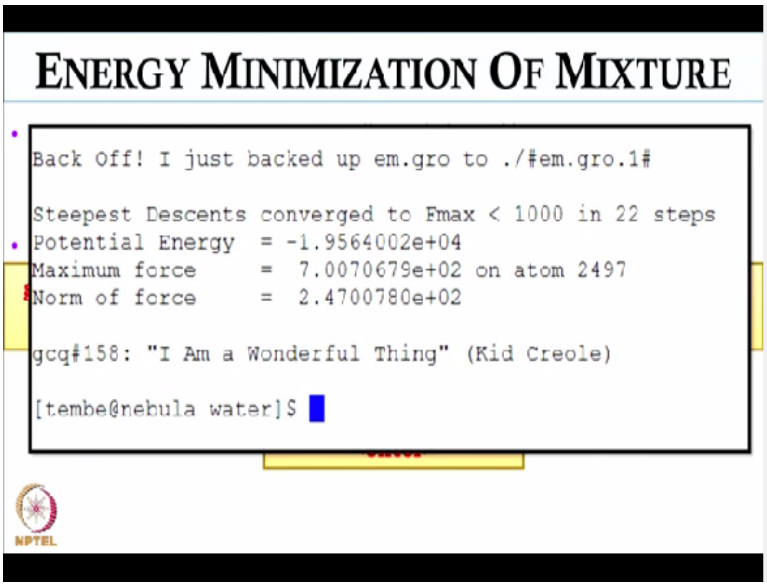

So after the energy minimization, we will have something like this displayed on the screen where we see potential energy is negative. Maximum force and normal of force is found to be there. So

this time also it has taken 22 steps? Yes. Last time also 22? It depends on the system also. Okay. If you have a large system, it is just, see because the number of, total number of molecule here is 862. Right.

In case of water, we have taken 899. Okay. So it is very close? It is very close. So if you have a large system, suppose 4000 molecule, then it will take. May be a longer. Longer time or longer step. So now instead of writing something after 22 steps. Yes. Can I write that force every step? Yes, it is displayed on the screen, force on each step is displayed on the screen. Or is that also written into a log file?

Yes, em.log file will be generated. You will have force as a function of time, as a function of step. So whatever is happening every step, that is written into a log file. Yes, definitely. So is there a log file for every execution? Yes, there is a log file for every execution. For energy minimization, you will have em.log. Okay.

Then when you do full molecular dynamics simulation, you will have full.log. Okay. And many of these things in the log file also will be on the screen. Yes. If you are doing on the screen. Yes, yes, yes, sure. Okay. So now again the maximum force is of the order of 10 to the power 2 on atom 2497. 2497. Okay.

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So now since we have energy minimized configuration, we have the topology file and we have the full.mdp file. So we will proceed towards the molecular dynamics simulation of the mixture. So here also we will combine the mdp, em.gro and topol.top file to a tpr file which will be my input for mdrun using the command grompp. So em.gro is the result of? Energy minimization. Energy minimization.

So that is a 1 file? Yes, that is 1 file. Okay. Consists of all the coordinates? All coordinates of methanol and water. This is the energy minimized configuration. Right. And we will use full.mdp which contains detail information about algorithms, like which is the algorithm we are using for keeping the velocity, sorry temperature constant, for pressure constant and how many steps. So that full.mdp? Yes.

That we are using here, is it the same that we use for water? Yes, you can use the same mdp file. Okay. I will also show the details of the mdp file when we actually do, run the simulation in lab. That mdp file here. Yes. Should it not contain parameters for methanol as well as for water. No, no, no. For water and methanol, we do not need different parameters. What is in the mdp file, is the number of steps.

Okay. It is the time steps. Then after how many steps you want to save your coordinates, velocity, force, trajectory and then. So the mdp file. Cut off. So it has nothing to do with the types of molecules. No it has nothing. It just has a global information of the system. System. Okay. Yes. And the gro file will have only the coordinates? Yes, gro file will have only the coordinates. And the box length.

And box length, yes. And your topol.top will have all the parameters. All the parameters, charge, mass, sigma, epsilon. And that connectivity, that is also in topol.top? Yes, that is in topol.top. That is, itp file is included there. In the top, okay. In the itp file, it is there. So your full.tpr will be the output of this.

grompp command and it will contain all the information which is contained in the mdp file. Okay. gro file and top file. Okay. And so now we will use this tpr file for mdrun. So we will type

mdrun -v -deffnm full. So all my output file generated will have initial as full. So full.gro, full.xtc. Right. So like this.

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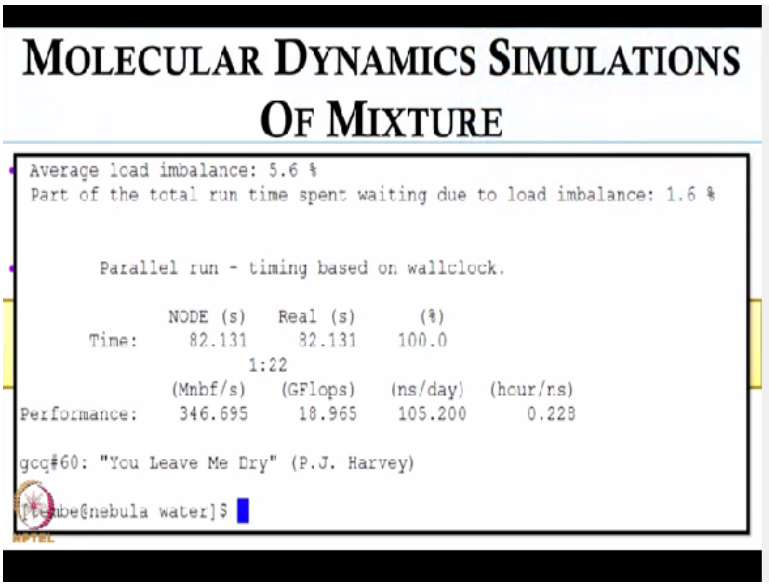

So now since we are done with the simulation, so something like this will be displayed after you are in the simulation. So does this display include the number of step or not? No, no, no. It does not include the number of steps. So that will be in the log file. That will be in the log file. Okay. Your temperature, pressure at each and every time step, that will be contained in the log file itself. Okay. That will be full.log.

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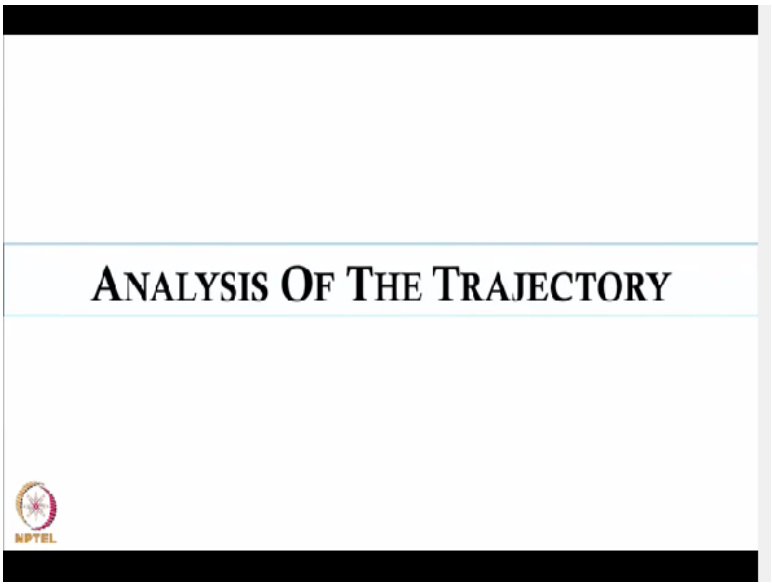

So now we will proceed towards the analysis of the trajectory. So here also we will go first

creating an index file.

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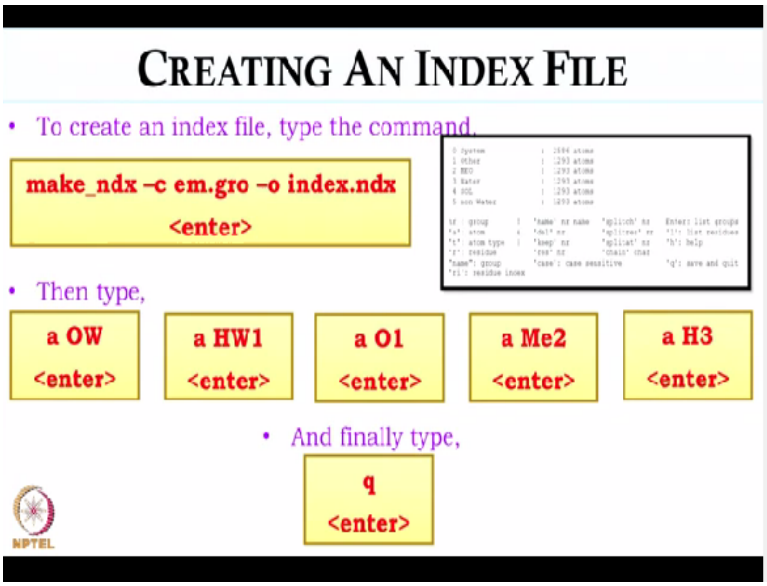

So to create an index file, we will first type the command make_ndx -c em.gro. Similarly, here we can use any gro file. We can use full.gro or we can use conf.gro. Then space -o, -o is the output file name. So all those gro files will have the same index? Same index, yes. Okay. And then -o index.ndx and then when we type enter, something like this will be displayed. So here we see there are 5 default index groups that are already created.

So the first default group is system. That will contain total number of 2586 atom. It will contain all methanol and water molecule. Then there is. So the index is index of all the atoms? All the atoms. Okay. Yes, then there is other. Other will contain the index file of all methanol. Okay. Then meo... But if you had given water first and then methanol, the other would contain water first?

No in case of water, we have water and sol. It will have water. Because in the data. Yes. We had given methanol first. Yes. So the output, that index file output is the same for all systems. Yes, it is the same, like it will have one system. Then it will have 2 for like, it would have 2 for methanol, right. 1 is system. Right. Sorry 1 is other and 1 is meo. Since meo is the residue name that we are giving. Okay.

Then there is 2 for water. Okay. Water and sol. Then there is non-water. Non-water is also methanol. Okay. So these are by default created index file. We cannot change this. It is created by default by the system. So every time you do that, make index, it will create that file? It will create that file depending on the molecules of the system that you are simulating. Suppose I had given only water?

Only water, then it would have system. Right. Water and sol. Sol is the residue name. Okay. So it would have 3 index files. So if you have 3 solvents, you will have? May be 9 or 10 or may be more than that. But there we have no choice? There we have no choice. We cannot change it. We cannot edit it. So that is the system output? That is the system output. It is created by default. So now to make indices for all your atoms, you have to give that a...

Yes, yes, yes. Right. So now since there are, in water, we have 3 sites and 2 hydrogen sites are equal. Okay. So we will just create 2 for water and in methanol, we are using united atom for the methyl group. And oxygen? And oxygen and hydrogen. They are different, so you will have 3. 3, 3 for methanol and 2 for water. Water, okay. So we will first type a OW, then enter. So this is before that q comes?

Yes, this is before that q comes. Okay. Then we will type a HW1. Okay. This is for water and then for methanol, we will type a O1. Okay. Then a Me2 for methyl group. Okay. Then a H3 for hydrogen and then finally to save it, we will type q. q, so now that HW1. Yes. It is just the name you are giving. It could be HW2. Yes, it could be HW2 but it has to be HW1 on HW2 for water. Okay. Similarly, for methanol since in the pdb file, it is already O1, me2 and H3.

So we have no choice. We have to give O1. We have to give me2 and we have to give H3. Okay. We cannot write H4 or H1 or H2. So now is the order of these commands important? No it is not important. So I can do a H3 first and then a Me2? Yes, yes, yes. Then a OW, I can mix them all? Yes, you can mix them all. Basically I will give 5 commands. To generate. To generate indices for this file. Yes. So what is the output file of aaw.

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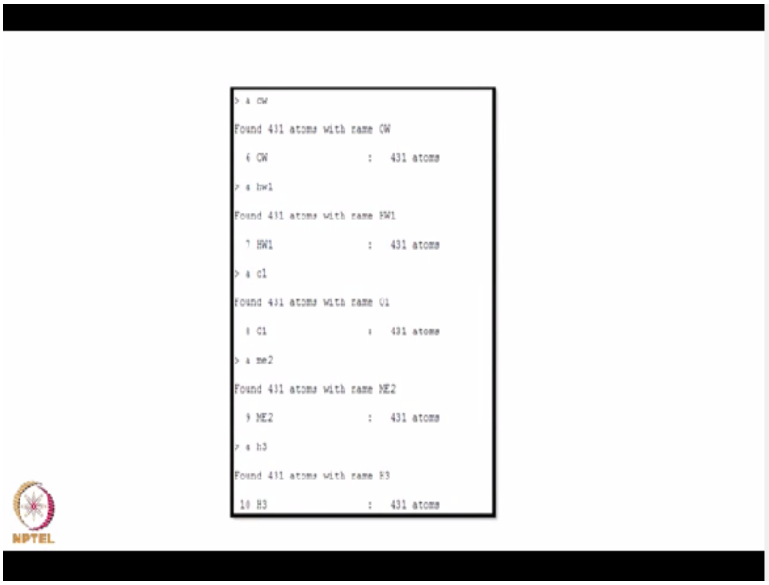

Yes, so when you type all this. Yes. You will get like this. So there is like, there is already 5 default index files created. So the sixth one will be for OW. So 6OW, there is 431 atoms, right. Okay. Then seventh is for HW1, that is 431 atom. Then eighth is for O1 of methanol. Again 431. Then ninth is for methyl group of methanol, 431 atoms. And then tenth will be H3 of methanol, that is also 431 atoms.

So when you open the file using the command vi index.ndx, you will see all the index file, like first will be 0 like it will contain system. Then there will be 1-2586 atoms. Okay. Then when you go to OW, it will have 1-431 atoms. So whatever was in your default file that you showed. Yes. Plus these will be in your index file. Index file. Yes. Okay. So now we have index file, we have xtc file and we have tpr file. Okay. Right. So now we will use all these 3 files to create, to calculate radial distribution function and diffusion coefficient.

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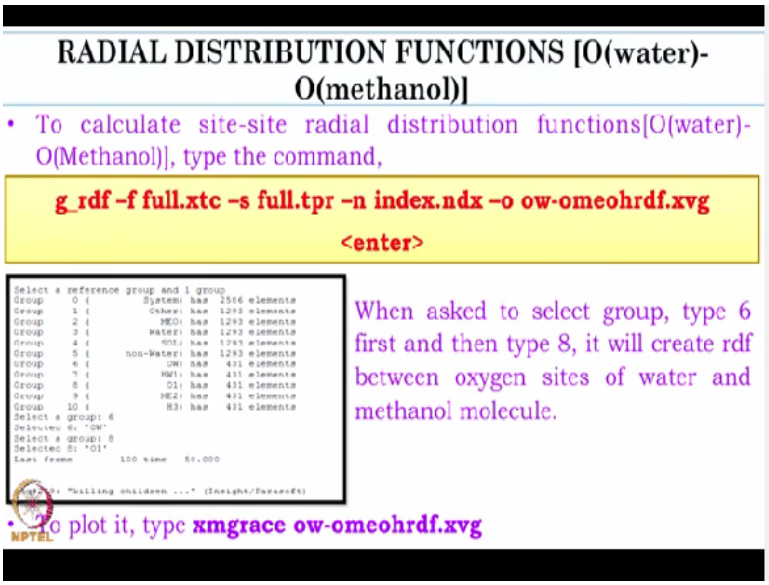

You have a printout of that index file total. Yes, we can show it. Okay. In the next lecture may be. Okay, fine. So now to calculate radial distribution function between... But just as your pdb file. Yes, yes. Or your topology file. Yes, you can create it by yourself packing all those things. You can actually type on the screen. Yes, but, yes, yes, yes. It may take time. It will take long time. Same way, if I know what my system is, can I create that index file, since I know all the atoms, all the molecules.

Can I create that index file by hand? Yes you can create it by hand but it will be a, it will take long time because you have to specify each and every atom number has to be written there. So if you have more than... No, no but you said that the index file will have 10 lines. No, no, it will not have 10 lines. Oh, it will have an index for every atom? Yes, it will have an index for every atom.

Okay. So to, now coming back to radial distribution function, so we are calculating between oxygen site of water and oxygen of methanol. So we will use the same command g_rdf and xtc, tpr and index file are the input to calculate radial distribution functions. This is exactly like the same. For water. The commands earlier. Yes. Okay. And then -o space whatever the output file you want to give.

Okay. So I have given your ow for water and omeohrdf.xvg and then it will ask you to select a group. Okay. So here you have to select 2 groups, right. So first you will select oxygen of water.

It is in, see group 6, right. Right. And then oxygen of methanol is in group 8. Okay. So first you type 6 and then you type 8. Then it will create an rdf file, like rdf.xvg file. But when you type that first line.

Yes. One in red, does it prompt you to type a particular group? Yes, it prompts you to type a particular group. So type group 1. Yes, yes. Group 2. Yes. It will give you that. Yes. Okay. You see here it is written select a reference group and 1 group. Okay. So around which atom you want to... Correct. Know the density or... So first you select a reference group. Yes, yes, yes. And second time, 1 more group. Yes. Okay. So after that you will have a file owomeohrdf.xvg, you can view the file using the command xmgrace. Okay. So just type xmgrace space the file name.

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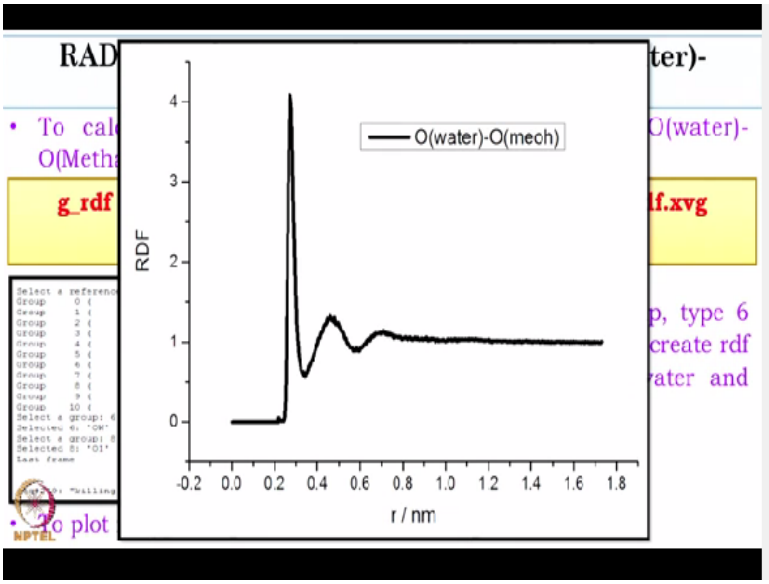

And then it will show the graph as this. Okay. So O water, O meoh, you have the 6 and 8. 8, yes. Okay.

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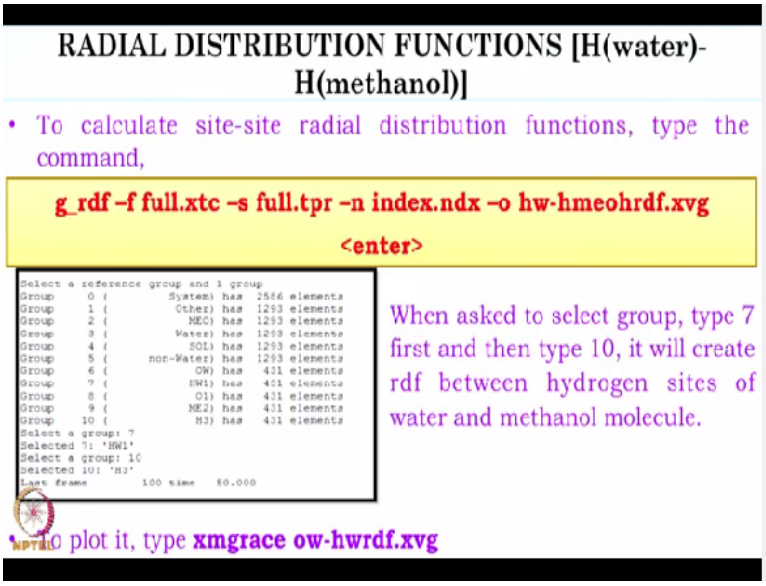

And now for hydrogen of water and hydrogen of methanol, we use the same command, just give the file, output file name different and then here what we do, since hydrogen of water is required, so hydrogen of water is in group 7, right. Okay. So you type 7 first and then type 10 later because 10 is hydrogen of methanol. And then you will have the file o hydrogen in water, hydrogen in methanol rdf.xvg. you can plot it using the same command xmgrace. Yes.

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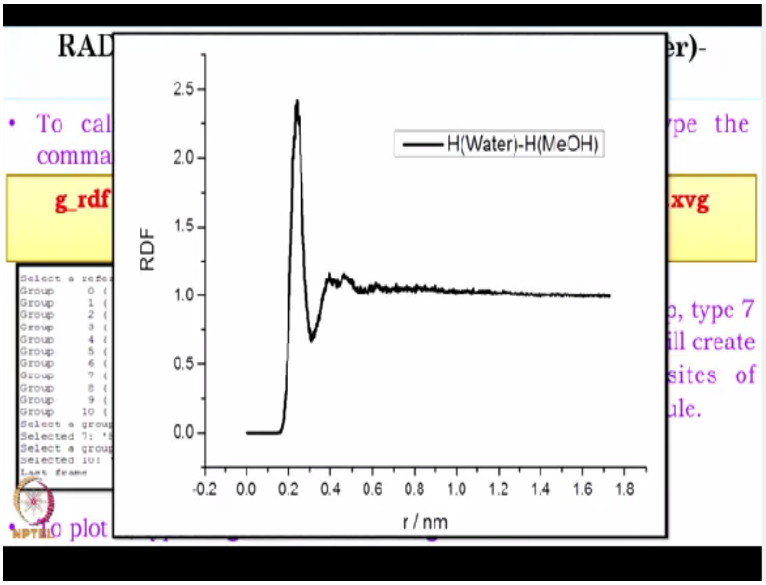

So it will show something like this. So basically you can choose any pair. Yes. And get all the distribution functions. Yes, so. You can also get H water H water also. Yes, H water H water. So use the same index? For H water H water, you have to give like water is in group 7, right. So you have to type 7 twice. Okay. For getting gfr between water of, hydrogen of water molecule. Okay.

So now we will go to diffusion coefficient of water and methanol.

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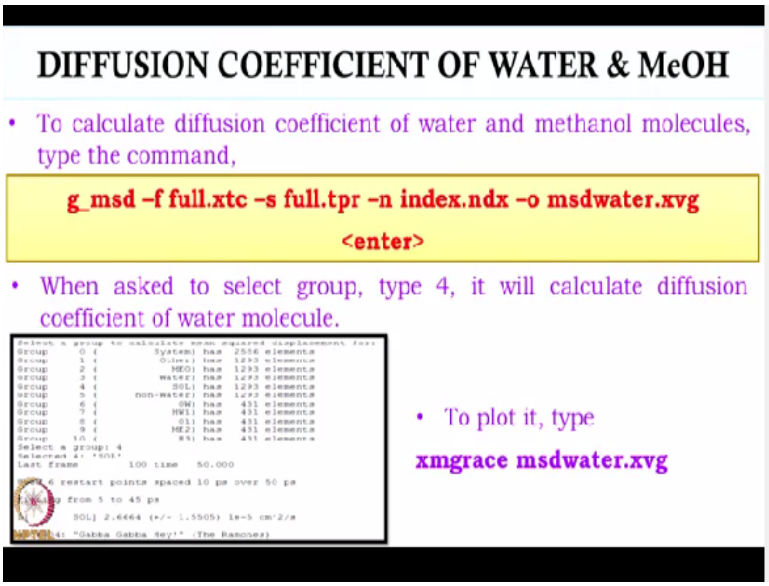

So we will use g_msd, same xtc, tpr and index file is required and -o msdwater, since I will first calculate the diffusion of water molecule. So this is the output file name and it will... So is there some way where I can include all those files in one command -f full.xtc -s full., every time you have to type all that. Yes, every time you have to type all that. Is there a way to put that on in some shortcut?

No, no, there is no shortcut there. Or can I not create a shell script for that? You can create. Very simple. Yes, you can create that. Right. So that shell script you will give input. Yes. You will only need that output as the msdwater.xvg. xvg. That is the only thing that is changed. Yes, yes, yes. All the rest are the same. Yes. So there must be some way. Yes, you can write a script file as well. So you do not have to type it again and again.

Correct, okay. And it will also ask to select a group for. Diffusion. Diffusion. So here we have to calculate diffusion for the whole molecule. Okay. Right, so for, if you want to calculate for water, so what we do here is, yes. You have to select that group. Yes, we have to select a group. So you see in group 4, there is water and sol. Okay. Water is in 4 and sol is in 5. So you can type either 4 or 5. Okay.

It will display the diffusion coefficient as shown in the screen. And to plot it, you just have to type xmgrace space your file name.xvg. So now to calculate the diffusion coefficient of hydrogen, you can give that site also? Yes, but there is no meaning of calculating diffusion of different sites, like the molecule will diffuse as a whole. I understand. So whether you do for O or H, they should both diffuse with the same diffusion constant.

Yes, they should in principle. But this so, how does the system decides that the oxygen is the main atom or that is built in to the system? That is built in because oxygen is a center of molecule. Okay. So for oxygen, it will be for water and similarly for methanol also. Yes, for methanol also like we use the same command. Right.

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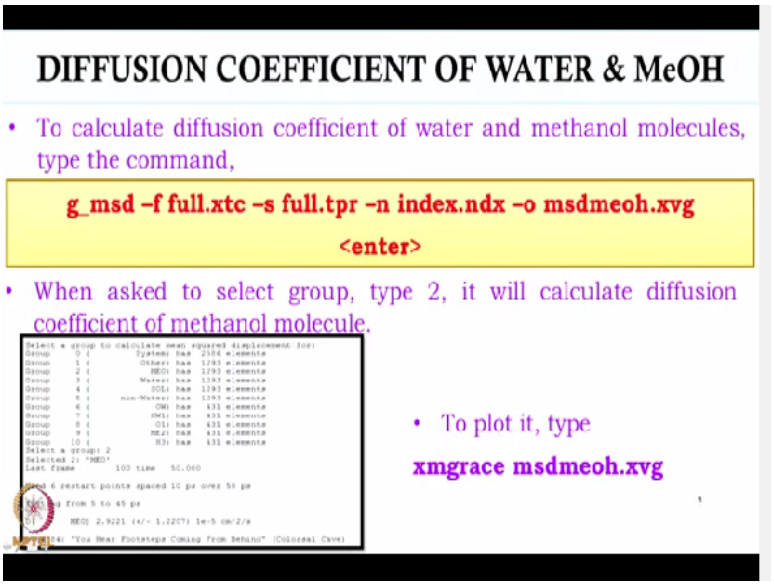

Just we will give the name of the output file different. Different. And then for methanol, we type, we just have to see methanol is in group 2, right. Okay. So we just type group 2. Okay. Like we type 2 and then we will get the value of diffusion coefficient on the screen. Okay. And we will have the output file as xvg and to plot it, we just type xmgrace output file name.xvg. Okay.

So now we have completed the calculation for a mixture. Yes. So we have done all the file structure, all the commands, these are all done. From next time, we will actually do the practical part. Right from installation to execution of all these things what we have studied so far. We will close here and see you next time. Thank you.