Computational Chemistry & Classical Molecular Dynamics
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Lecture – 37
Molecular Dynamics using Gromacs-5: Liquid Water: Analysis of Results

We will now continue our discussion on simulation on water. So far from the PDP file for water, we have come up to the configuration.gro file. So let us continue with that conf.gro file. We talked that this file will have the coordinates of all the water molecules. We have 899 molecules and 3 times 899 is 2697. All the coordinates are written from third line up to line number 2699. Would that be the last line or? Yes, that would be the last line and the last line will be the box length also. Okay.

What is the format on that last line? The last line, the format is in nanometer, 3.0 3.0 3.0.

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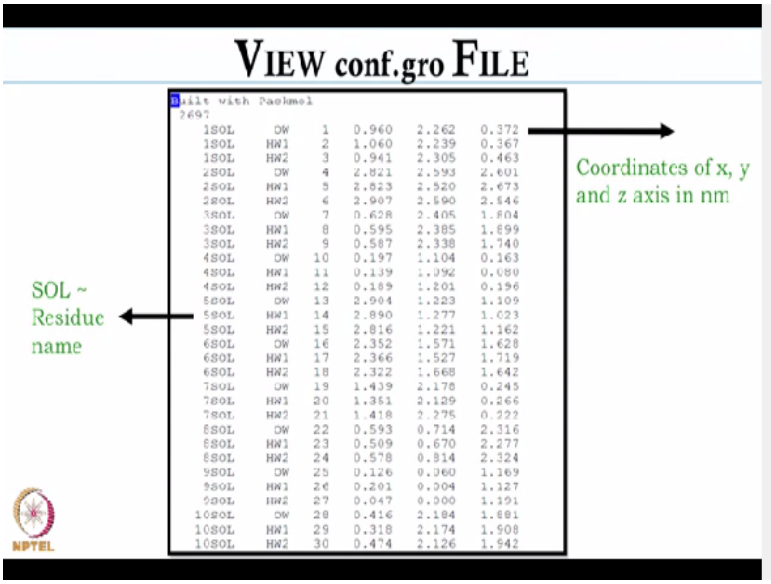

This is the format of the last line. And so on the last line, there will not be this 6 SOL 6... No, no, no, no, no. It will just x, y, z or not x, y, z; the box size? Yes, the box... Dimensions. Yes. Okay. So what is the next step now from the, you have a file.

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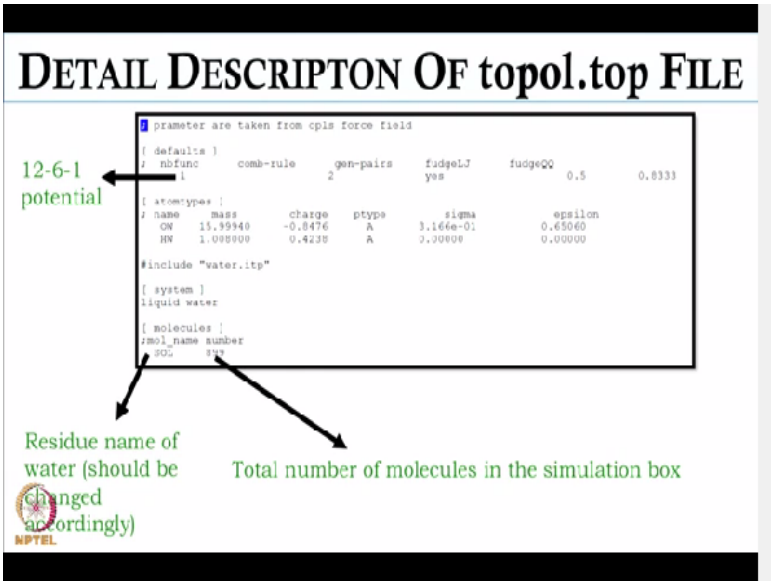

The next step is we have to have a topology file for water. Okay. Because it will contain all the force field parameters, sigma, epsilon, charge and mass. Okay. So this is the topol.top file for water. Okay. So here same thing and nb function as I have already said earlier, if it is 1, it corresponds to non-bonded function and it corresponds to a 12-6-1 potential. So it can be changed according to the user, whatever they want to, potential they want to use.

Now this topol.top files, are they available on websites or they have to be created. Yes, yes, they are available on website and you can create it as well from, if you have your PDP file. Okay. Of any molecule that you want to create a topology file of. Okay. Suppose you want to create a topology file of water, so you have the coordinates. You have the OH bond length and bond angle.

Okay. So you have to enter the bond length and bond angle in aminoacids.rtp file. Okay. This is a file which is contained in OPLS folder. Okay. And this is a folder in top folder. So top will be automatically downloaded when you install Gromacs. Okay. So it will have all the force field directory, CHARMM, AMBER, OPLS. Okay. GROMOS force field. Okay. So whatever force field you want to use, say OPLS or AMBER.

Suppose you want to use OPLS for water, so you have to go to the directory OPLS. Okay. There there is a file aminoacids.rtp. Okay. You open the file using the command vi, go the last line. Just

write the residue name of water. Okay. And bond length and bond angle. Then you have to use the command pdb2gmx. Okay. And then input will be your PDB file and output will be your topology file.

Okay. So may be when we install Gromacs, show them installation, we will show how to create a top file. Yes, yes, yes. We can show them. Not only from the data that is already there but also we can create our own. Yes, yes, we can create for ethanol or methanol or some complicated molecule as well. Okay. So the first line is common parameter or that is just like comment here? The first line is a comment here that parameter is taken from OPLS force field. Right.

So it is the fourth line, 1 2 3, fifth line really is the actual data. Yes. The first default is part of every file. Yes, default is part of every file. Okay. So non-bonded function depends on the user which potential they want to use. Okay. Then there is combination rule 2. Combination rule 2 is not coming exactly below that comment. Yes that does not matter actually. So it can be anywhere it like.

It can be anywhere in that line. Okay. Then there is gen-pairs, yes that will generate interaction between 1-4, 1-4 interaction will be generated. Okay. If you give yes, and... What is the meaning of this 1-4? 1-4 is long range interaction between water molecule. So since in case of argon, you do not required it but water since it is a triatomic molecule, so you may as well give yes to generate the interaction, long range interaction.

No but in case of water, you had 3 atoms. Yes. Right. Now naturally anything 1-2, 1-3 is part of a given... Part of a given molecule. So 1-4 is outside the first molecule. Outside the first molecule. But suppose instead of water, we have methane. Yes. So methane will have 5 atoms. 5 atoms. So do you call that interaction between 2 methane as 1-6? 2 methane 1-2, but it is not, it depends on which atoms you are counting, alright.

Okay. But see, just as for water I have OHH. Yes. So in methane I will have CH1H2H3H4. H3H4, yes. Right. So 5 atoms are for methane. So if I want between 1 methane another methane. Yes. You may call it 1-4 as a nomenclature. Yes. But in reality it is 1-6. In reality it will be 1-6.

Okay. So when you say yes for gen-pairs that means it... It will generate... Intermolecular. Yes. Not intramolecular.

No and intermolecular will be when there are more than 4 atoms. Say in case of ethanol. Okay. There will be 1-4 interaction in case of ethanol. If it is a rigid molecule, there really should not be. Yes. But in reality, it is not a rigid molecule. The molecules are allowed to move. You just fix the, you can fix the bond length and bond angle but the molecules move in the simulation box.

They are not fix in some way. So it means 1-2-3, you do not want this to change but 1-4. Yes. You are allowing it to interact. Yes. And this fudgeLJ and fudgeQQ, these are the parameters to model this interaction. FudgeLJ is the Lennard-Jones parameter. Okay and fudgeQQ is the electrostatic interaction parameter. So this will model the 1-4 interaction. Okay. So that fudgeLJ, fudgeQQ is always for intermolecule fudge.

Yes. Okay. But why that fudgeLJ is 0.5 and the other one... The maximum value is for fudgeLJ and fudgeQQ is 1. Okay. So the maximum you can take 1, not more than 1. Have you tried other than 0.5 or 0.83. I have tried 0.6 for fudgeLJ and for fudgeQQ 1, and I have tried 1 for both. But it does not really change the interaction or the result. Overall results... The overall results are more or less affected by the sigma epsilon values and charge values rather than this.

Okay. fudgeLJ and QQ values. Okay. So that is the first line which tells about the interaction. Yes. Then 1 blank line and atomtypes. Yes. Atomtypes you have to describe the charge, mass and... Okay. You have to give the value of sigma and epsilon. Okay. So since there are 3 sites, oxygen and hydrogen and both the hydrogens are similar. Correct. So both will have same mass, charge for oxygen is -0.8476 and for hydrogen it is 0.4238.

Then sigma and epsilon for hydrogen is 0 and for oxygen, the value is 3.1*10 raise to power -1 in nanometer. Okay. And epsilon is in kilojoules/mole. Okay. So and now you should all notice that the charge on oxygen is -0.8476. So for each hydrogen, it is half of that. Yes. Because the sum of 2 hydrogen charges should be equal to... Equal to the sum of... Oxygen charge. So that the molecule is neutral overall.

Yes. Okay. That, what is that next line, it include water.itp. Include water.itp. In water.itp, we will have the bond length since in case of water, there are 2 bonds. Okay. So we will have to provide the bond length, bond force constant, bond angle, the bond angle force constant and if there is any exclusion like any interaction you want to exclude from your simulation, all results to be provided in the water.itp file.

But itp file, we had already created or we have to create now? Itp file you have to create now. It is not yet created. No. Okay. And then there is system, you have to define whatever system you want to simulate. Okay. And then there is molecule name and number. Molecule name you have to give the residue name. Okay. And you have to change the residue name accordingly in the topology file whichever molecule or atom you want to simulate and number is 899.

It is the total number of molecules which is taken in the simulation box. It is the same as before. We cannot change that. Yes. Like you have to change it according to the number of molecules you are taking. Okay. Whatever you are giving as an input in inp file, say if it is 900, you have to give 900 here. Okay. Or else it will show an error.

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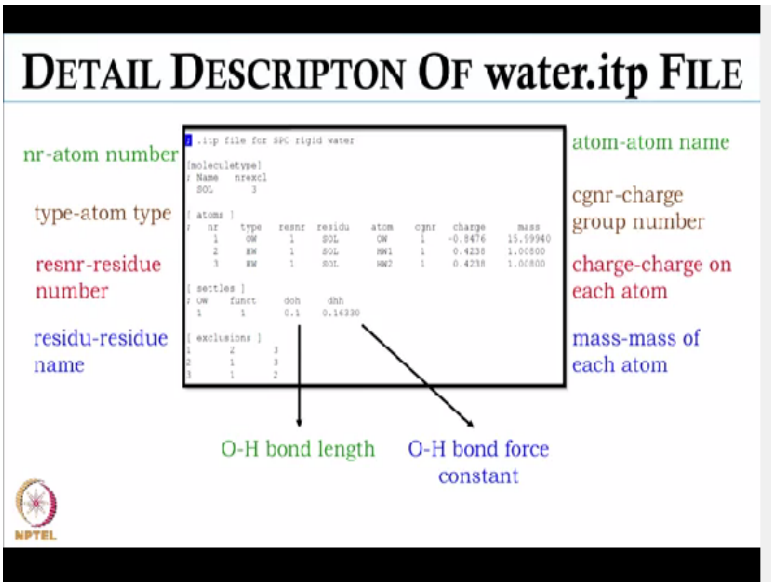

So now we will come to water.itp file. So there is the itp file format. Hit nr, so first you have to define the residue name of water. So that is s o l SOL, nr in atoms, it is the atom number. Since

there are 3 atoms, so it is 1 2 and 3. Then there is type which defines the atom type. No before that you have name is SOL. Yes. And nr? That is the excluded interaction. Okay. What is the meaning of that?

It is the number of interactions you want to exclude after certain atoms. Like after 3 atoms, you do not want to count the interaction. So if it is methanol, I will be, sorry if it is methane, will I be giving it as 5? Yes, yes. It will change from molecule to molecule. So it depends on the total number of sites on a molecule. Yes and which kind of, like if you are taking united atom or if... Then the size will be different.

Yes. Now what will happen if there is a mixture instead of a single molecule? There will be 2 itp files or only 1? There will be 2 itp files for 2, suppose there is water-methanol mixture. You will have to have a itp file for water and a separate itp file for methanol. So in this case both will be solvents but nrexel will be different for the 2. Yes. Okay. So then you have this... Type which is atom types.

If there are 3 atoms OW HW and HW, then there will be residue number. Okay. Okay, and there will be residue name. So which is s o l solvent. Then there is atom name. There is OW HW1 and HW2. Then there is cgnr that is charge group number. And then there is charge you have to define and then there is mass. Mass on each atom has to be written there. And then there is a function DH, DOH and DHH.

So this is the OH bond length in nanometer and then that is the OH bond force constant. And these are the exclusion. Now DHH is the force constant or the distance between hydrogens? Sorry DHH is the distance between hydrogen. So they can actually calculate it from the coordinates. Yes, yes, they can coordinate in calculation and DOH is the bond angle. That force constant you will mention somewhere else?

Yes, I will mention it. Right. Actually has to be mentioned in the itp file itself. Okay. So I think I have to change the itp file a little bit. I just have to add 1 extra column in that, after DHH itself. So to be on the force constant. Yes. Okay. So now what are the last lines now? Those are the

exclusion. When you create an itp file. Okay.

From a topology file, this exclusions are automatically created. If you do not give it as, it does not matter. So which means if I skip the last 3 lines, it is okay? It is okay. But you have to give the bond length, bond angle, that has to be provided there. So now we have itp file, topology file and we have gro file.

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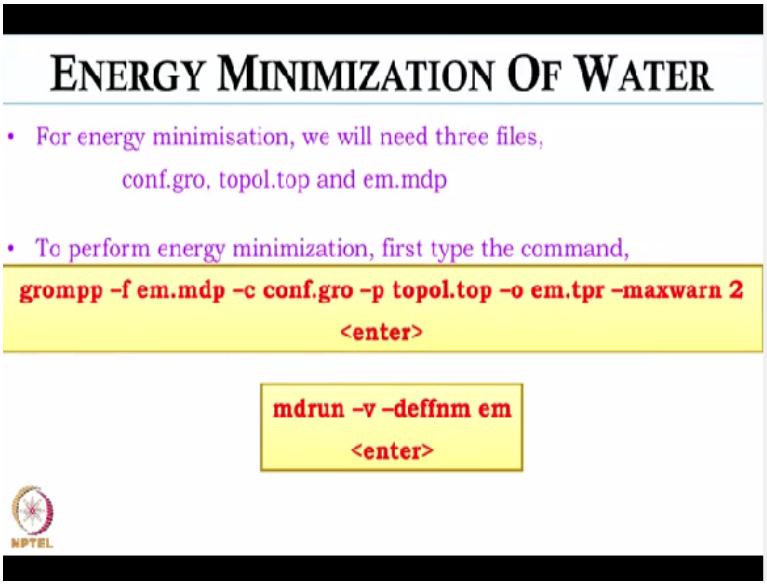

And ndp file is already there. Okay. So now we will proceed through the energy minimization of water. So these are the 3 files that are required, conf.gro, topol.top and em.mdp. mdp is for molecular dynamics parameter file and em is for energy minimization. So to perform energy minimization, first we have to generate a tpr file using the command grompp. So grompp -f em.mdp -c conf.gro -p topol.top -o, for output, em.tpr -maxwarn 2.

So it will generate a tpr file, em.tpr which will contain information about the mdp file, gro file and topol file and it will be an input for the mdrun. mdrun or minimization? mdrun for energy minimization. Okay. So next we will do mdrun. So mdrun -v -deffnm em. So it will create all the output file which will have initial as em. So the output file will be em.gro, em.xtc, em.ebr, em.log like this.

So whatever we will give the tpr file extension like em.tpr, in mdrun we have to give the same

name em. We cannot change it. So now the grompp, the output was em.tpr? Yes. For mdrun -v. Yes. What is the input for mdrun? em.tpr. em.tpr. Nothing else. Nothing else. Because the em.tpr contains all information about mdp. Yes. gro and topol. Okay and deffnm em means all files will have em as the initial.

Yes. And how many outputs does mdrun create, that you will have in the next slide? There are many output like you will have edr file, you will have energy file. Okay. You will have xtc file which will contain the trajectory. Then you will have gro file definitely which will be the energy minimize configuration. Okay. Then you will have log file. It depends on what are, what files you want to have.

So instead of mdrun -v deffnm, I could have given all the files name relevant to that? Yes, all the files name relevant to that but it will be a... Those will have different names now. Yes, but that will be a long command and it is easier to have it because then you will know that okay em.gro is the energy minimize configuration or if the file name is em.edr which will mean that it is the energy file for energy minimization.

So whatever you said now, if I say mdrun -h. Yes. It will give me all the details? Yes, it will give all the details. If I see the -v option. Yes. Then I will know what it is going to do. It explains that. Yes, it explains that. Okay. So after energy minimization is done, something like this will be displayed in the screen.

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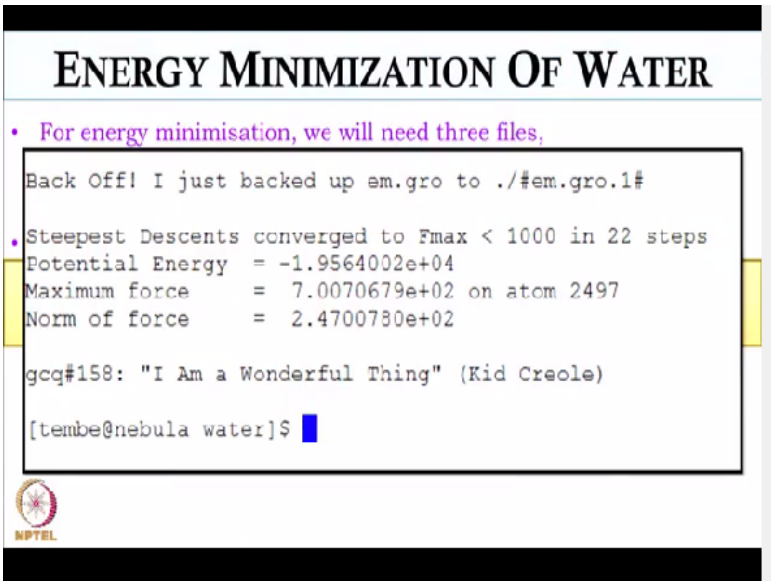

Okay. So you see that the steepest descents algorithm that we have already discussed in liquid argon. So here also we use the same algorithm for energy minimization and it is converged in 22 steps and the potential energy is negative in this case. Okay, first you have lots of plus minus interactions. Yes, exactly. And that < 1000 means, the maximum value of force is < 1000?

Kilojoule/mole/nanometer. Not angstrom? No. Okay. Everything has to be in nanometer. Okay. Distance, time has to be in picoseconds, energy has to be in kilojoules/mole. So now potential energy will be again kilojoules/mole? /moles, yes. And maximum force? It is not given in the units here. No. It is understood. Yes. Right. The maximum force is 7*10 raise to the power 2 kilojoule/mole/nanometer on atom number 2497.

And so what is the norm of the force? That is I guess the tangent of the force, I think so. Okay. So suppose I want to know the meaning of norm of force. You can get it. The manual will tell. Yes the manual will tell you what does it mean. Okay. So now we have the energy minimize configuration which we will use for our full molecular dynamic simulation. Okay, now all these files are saved in the water directory.

Yes, all these files are saved in water directory. And that is already under Gromacs? Yes. But why it is not showing that gromacs there because? Because I have done it in a different server, so. Okay. It is not showing there. But the water directory is in the gromacs? Yes water directory is in

gromacs. So when we perform simulations here. Okay. Then we will show them on screen. It will show as gromacs.

If you give pwd, we will get the path. So I will get the path here? Yes. So what will the path be like approximately? The path will be like who, then your name, then downloads in gromacs, then water. Okay. But how could all these things in downloads file only? Yes but it depends on you. You can as well change it from downloads to, you can create a folder name gromacs in your. Subdirectory.

Desktop or documents or downloads or in your hard disk and there you can. Okay, right. Install it as well. So now we have finished the energy minimization? Yes. Okay. And now we will use the gro file of energy minimization for full molecular dynamics. So what will be the first line? Go back, that ./emgro, what is the meaning of that? Okay, actually if you already have a file em.gro, it will overwrite the file to that. Okay. So that is the command. Okay.

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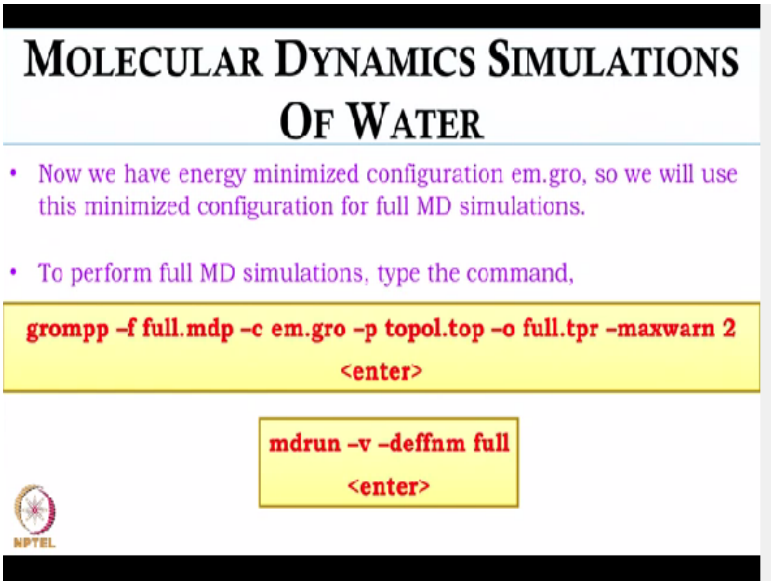

So for molecular dynamics simulation of water, we now have the energy minimized configuration, em.gro. Okay. We have topol.top and we have full.mdp file. Okay. So these are the files that are required. So we will type the same command to generate full.tpr file. We will use the grompp command and grompp -f full.mdp which is the molecular dynamics parameter file for full molecular dynamics simulation of water.

And -c em.gro, em.gro is the energy minimized configuration of water. Then space -p topol.top. So that will remain the same whether it is minimization? Yes, yes, yes. Or molecular dynamics. Because it contains the information about water. Right. So it is not going to change. What about full.mdp? That is different from. Yes that is different from minimized, energy minimization because in full.mdp, we will have detail about.

All information will be furnished. In which, some where you want to simulate. Suppose you want to do in a npt ensemble. So you have to fix the pressure, temperature. You have to use algorithms for that. Okay. And then since in this case we are simulating water also, you need to constraint the bond length and bond angle as well. Right. So we will have those constrained algorithm.

Those constraint are the same for your minimization also? In case of minimization, we do not actually use constraint. What... In case of minimization, we just have to give the algorithm name. Okay. Which algorithm name... So my minimization really does not change the bond lengths and bond angles. Yes. Because if it did that, there will be a huge problem. Yes. So minimization really calculates one energy, then use steepest descent.

Yes, yes, yes. It will go along some slope and get the lowest energy. Minimum, yes. Okay. So now this is, what is the end result of this, full.tpr? full.tpr is the end result of this and this tpr file we will use for mdrun. Okay. Just as in case of energy minimization, we used em.tpr for our mdrun. Right. So the command is same, mdrun -v -deffnm full. Okay. So it will create all the output file which will have full as the initial. File.

So now before we really go for the, what will be the main output files after this? The main output file will be full.gro. Right. And full.xtc. xtc file is the main output file because this is the trajectory file. Right. And this will be used in all the analysis. Okay. And now suppose at the end of the simulation. Yes. I want the last configuration. Yes. Where is that saved? That is saved in full.gro.

So full.gro has just one last... One last, it has one last configuration, so if you want to have the last configuration, suppose you have done, performed simulation for 10 picosecond. Okay. So you want to have the configuration for the 10th picosecond, right. So what you will do is you convert your xtc file. Okay. To full.xtc file to full.gro file. Okay. So just type the command, you have to use the command trjconv.

Okay. So it will convert your trajectory file to a gro file. Okay. So now your gro file will have configuration for each time frame. Like if you have given for 2 femtosecond as the time step. Okay. So at 0 time, it will have the configuration. Then after 2 femtosecond it will have configuration. So you have to convert your xtc file into a gro file using the command trjconv and then you will get the configuration for the last 10 picoseconds.

At each time frame, we will have configuration. But suppose I want just the last configuration? Still you have to convert it using trjconv. And then remove all the things except the last. Or you can just copy the last configuration in some other folder. But there is no automatic way of doing it? No, there is no automatic way of just getting 1 configuration, 1 time frame configuration. You have to convert the xtc file.

Okay. Suppose you want to convert the, you can give the beginning time and end time but it has to be between some time frame. So suppose my beginning time and ending time is the ending time? But then the simulation will not run. It want, the command. No, no. The command will say that your beginning time and end time is similar, so it cannot execute. So suppose you give the beginning time as 9.5 and end time as 10.

Yes, no problem. No problem. It will work. But your beginning time and end time has to be different. But as long as there is 1 delta T between, that is okay. Yes, that is okay. So I will be able to get 2 configurations, not 1. Yes, yes. Okay. And we will have different bonds length. Can you restart your simulations from the last configuration? Yes, you can restart simulation from your last configuration.

Suppose it has crashed, so you will have a cpt file. Okay. And you can restart it. Okay. I will

show it basic. Yes, when we will stop, we will see that. Yes, we will. So now since we have performed full molecular dynamic simulation and we have full.xtc file, so we will proceed towards the analysis of your trajectory.

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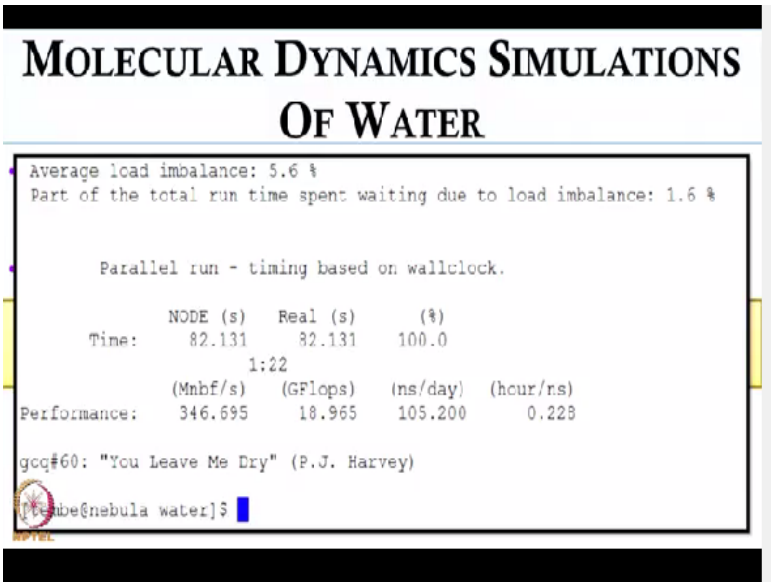

So after the end of the simulation, something like this will be displayed. So 1.22, 1:22 is the time that is required to finish the simulations since it is just 20 picoseconds, so it took 1 minute 22 seconds to finish the simulation. On a big machine, on a... Yes. On a PC, how long will it take, roughly? Depends on the system actually. Okay.

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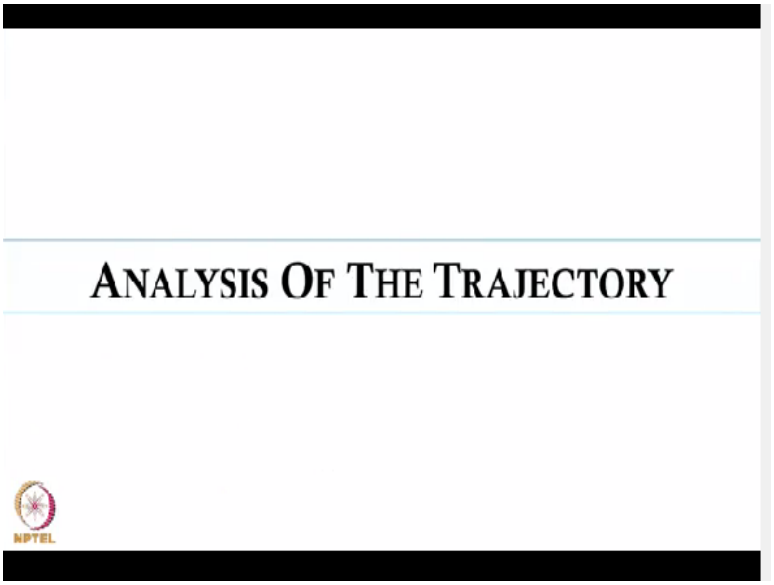

So now we will analyze the trajectory. So first we will see the, first since in case of water, we

have 3 sites, so we have to create an index file in this case as we did in case of argon. So to create an index file, we have to type the command make_ndx and then we have to use gro file.

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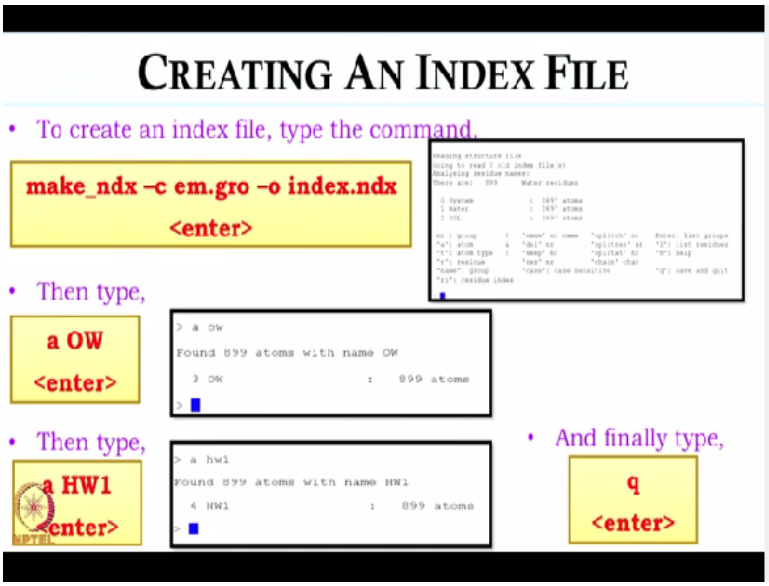

We can use any gro file, like conf.gro or em.gro or full.gro. Any gro file will work. And then space -o which is the output file command, space index.ndx. And then when we type enter, something like this will be displayed where there will be system water and sol. Okay. So since there are 3 sites, so we have to create index file for each and every site. Okay. Right, so to create index file for say...

No let us, whatever is on the right side. Yes. Comment more on that index file. Okay. So see there is by default if we just type the command make_ndx -c em.gro -o index.ndx and then if we type q, it will just save and exit the file and by default there will be 3 index files created. One is the system, one will be water and one will be sol. So all the 3 files are saved. Okay. But now since we have 3 different site in water, we need to create index file for all these 3 sites because we will calculate radial distribution function, right.

And we will calculate the site site rdx. Correct. So we need to have index file for different site as well. So to create... So whatever box you have shown on the right. Yes. Is that index file. That is not an index file, that is just a command you have given and after that command, this will be displayed on the screen. Okay. That is just a display screen. Yes. So now if you want to just save

and exit.

Okay. You just type q. Okay. Now if you want to create index file for different site, suppose you want to create for different atoms in water. Suppose I want oxygen and water. Yes, so then you have to type a, a which means atom type, then space OW. Oxygen of water. Yes. So which means whatever is on the right side of the screen. Yes. When you type the make_ndx, execute that.

Yes. That will appear. You have to type q to come out of it. Yes. Then type a.W. No, no. If you just type q, then it will come out of that. Correct. But then, first you have to type, but then if you want to create index file for a separate site. Right. You do not type q initially. First you type atom type OW, a OW, then something like this will be displayed. So found 899 atoms with name OW.

Okay. Right, because. Because there are 899 oxygens. Yes and then you... So which means after you execute make_ndx, you have to do that a.W. a OW. OW, okay. Then we have to, then there is hydrogen also. So you type a HW1. a is for atom type. Okay. Right, it will again display something like this. Okay. Found 899 atoms with atom name HW1 and since both the hydrogen atoms were similar, so you do not need to create 2 separate index file for 2 hydrogen.

Correct, now see it says 3 OW 899, first box. Because first is, first atom is one will be oxygen atom, so. Okay. And then finally, you type q and then enter. It will save and exit the file. So in the 2 boxes in the middle. Yes. It says 3 OW on the top and 4 HW1 at the bottom. Yes. So that 3 and 4, what are the meanings of that. 3 is the index file for 1 oxygen. The 4 is the for the fourth hydrogen.

Then 5 if you type a HW2, there will be 5HW2. Because 3 4 5 base will be the sequence. That is not clear. Can you clarify that a little better. Okay. Found 899 atoms with atom name OW. Okay. So 3 OW, 3 is the, like see, 0 is the system, right. Okay. 1 is water, 2 is sol, sol is the solvent. So third index will come as oxygen of water. Okay. This is the, this will come 3OW then space 899 atoms.

So after 0 1 2, you will have 3 as OW, then you will have 4 as HW1, then if you want to create

another index file for HW2, you will have 5HW2. So when you analyze the trajectory file, suppose you want to calculate a radial distribution function. When you type the command g_rdf, you will get a display of 5, like, what do I say. 5 separate files, like residues. First 0 will be system, then 1 will be water, 2 will be solvent, sol. Then 3 will be OW. 4 will be HW1, like this. Okay. So when we go for rdf, we will see the index file what 3 and 4 actually means.

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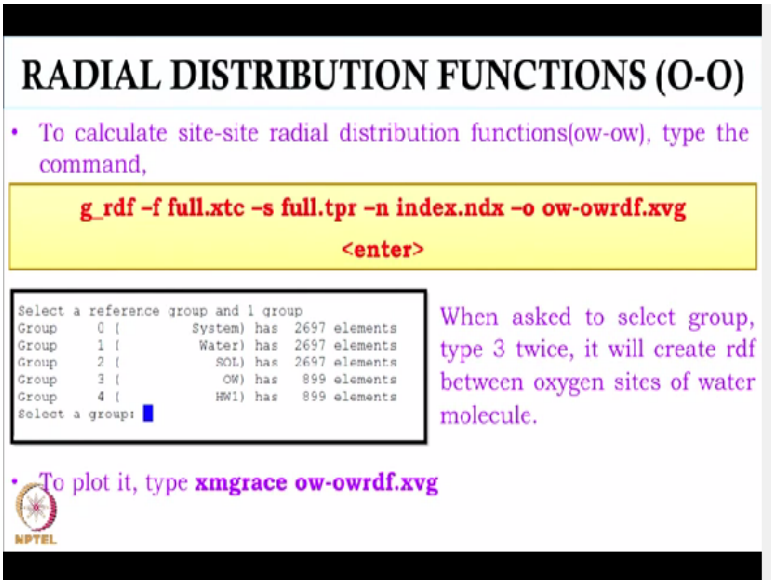

So now we have index file. So now we will calculate radial distribution function between oxygen site of water molecule. So to calculate, we have to type the command g-rdf, rdf means radial distribution function, and there are 3 input files that are required for each and every analysis. First is the xtc file, second is the tpr file. Okay. And third is the index file, right. Index file we have just created. tpr file, we have and xtc file, we have already in the folder.

And then -o is the output file, space ow owrdf.xvg is the file name of the rdf file. ow means we are creating. Oxygen of water, oxygen of water. Yes. But that could be any name? That could be, yes, yes, yes. That could be any name. That depends on the user what he or she wants to give. It could be just a.xvg? Yes, it could be that. So after you type the command, you will have to select a group.

So now you see there is 3 and 4 coming here. Okay. So that 3OW 899 was that in index file, the third index is for oxygen of water and the fourth index is for hydrogen of water. Okay. So that is

what 3 and 4 meant previously. Okay. Okay, so now since you have to calculate... But for 0 1 2. Yes. It is showing 2697 Yes, because they are total number of sites in the system, like. Okay. Since there are 899 water molecules, so it will have 2697 sites.

So it is containing the overall system. Okay. And now we have created for different site. For OW and for HW1. So it contains 899 and 899 water and HW1. Okay. So now to create a radial distribution function between oxygen of water, first we have to type 3 and then again, we have to type 3. Because we are creating gfr between. Oxygen and oxygen of water. Oxygen and oxygen of water. Okay. And now to view the file, you have just to type xmgrace space the xvg file name. Okay.

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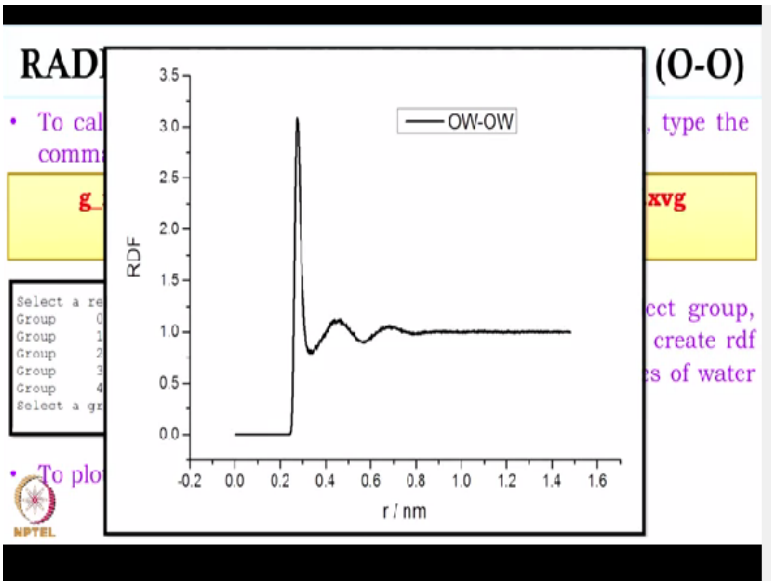

So it will automatically come up in the screen as, it will be displayed in the screen. So this is the radial distribution function between oxygen site of water molecule. So you have to type that 4 two times. 3 or 4. So. Type. Suppose in 3, group 3 is the oxygen of water. So once I select the group, you have to type 3.

And then again it will come select a group, you will have to again type 3. 3, so it will give oxygen-oxygen. Yes, it will give oxygen-oxygen. So this is the graph. Okay. X axis is the distance between oxygen-oxygen and y axis is the rdf. Okay. Now if you want between oxygen and hydrogen?

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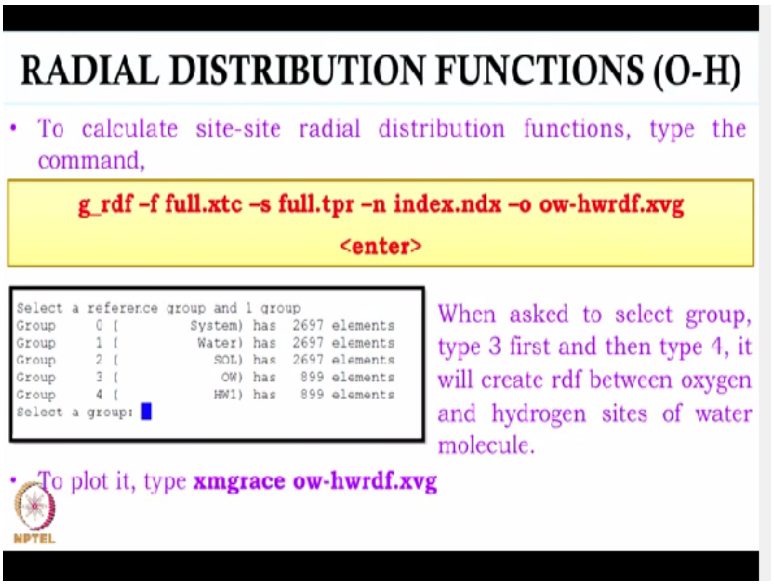

So between oxygen and hydrogen, we have to type the same command. Okay. Give the output file name different so that we can distinguish it. Right, okay. And then when it asks to select a group, so first you need to select oxygen, that is group 3 and then you need to select group 4, that is hydrogen. Okay. And now to plot it, just type xmgrace xvg file name. Okay.

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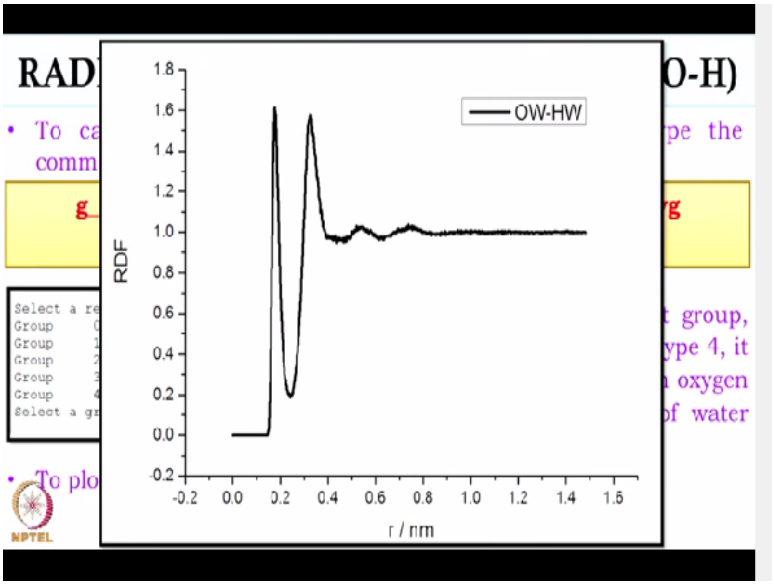

Right, so it will give the plot like this. Oxygen of, oxygen and.. Oxygen and hydrogen. So for hydrogen-hydrogen, it will be 4 and 4.

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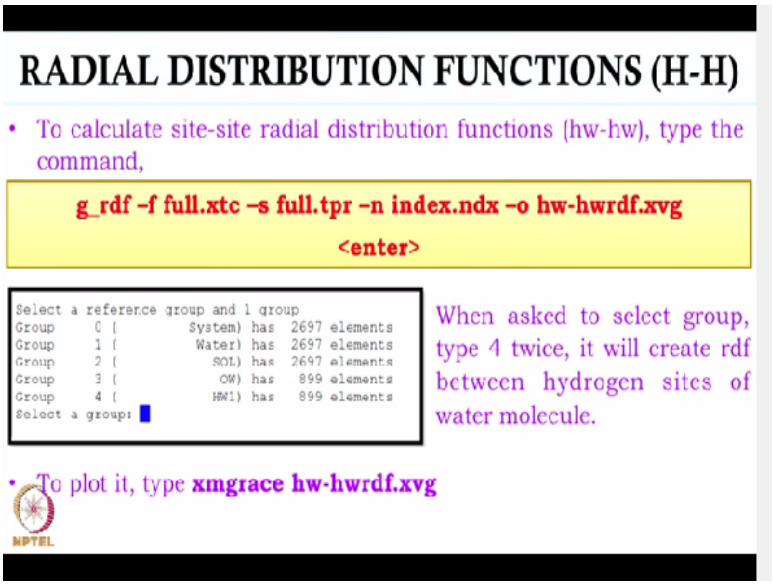

Yes, for hydrogen-hydrogen, same command. Yes. Output file name has to be different and you have to type group 4 twice. Okay. So 4 has to be typed twice. Yes.

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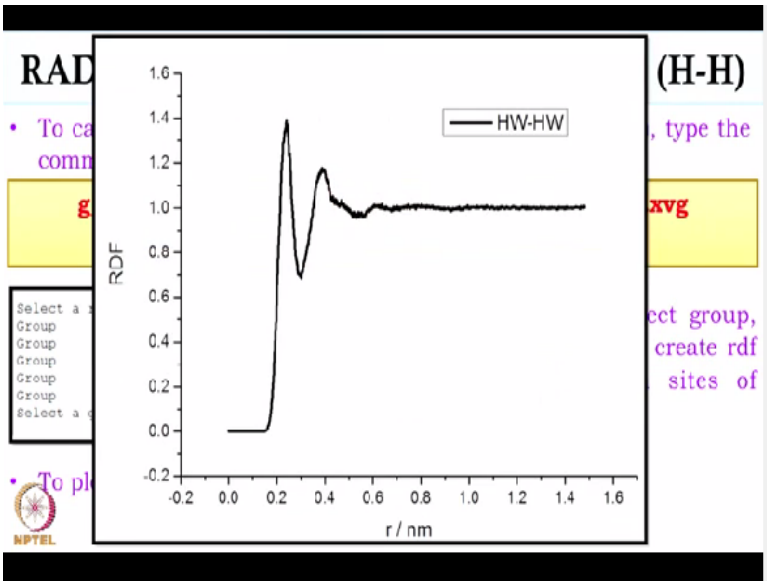

So now since we have to conclude in 2 to 3 minutes, can you show the diffusion behaviour also. Yes.

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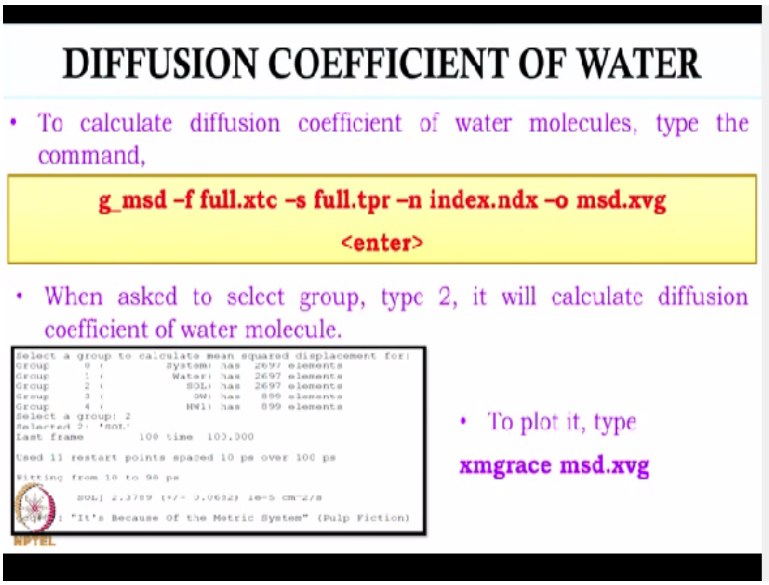

So for diffusion, we have to use the command g_msd, msd is the mean square displacement. And the other 3 are the same? Other 3 are the same. The last one is different. Last one is different because last one, this is msd.xvg. Right. So when you type it, you will have, you will again be asked to select a group.

So you type 2 or 0 or 1 because we do not want diffusion for a particular atom. Okay. We want diffusion for the whole molecule, right. Okay. So you just type 2 or 0 or 1. So it will display the diffusion coefficient value on screen which is 2.3*10 raise to the power -5 cm square/second. Okay. Within bracket is the error bar and if you want to view the file, you just type xmgrace msd.xvg.

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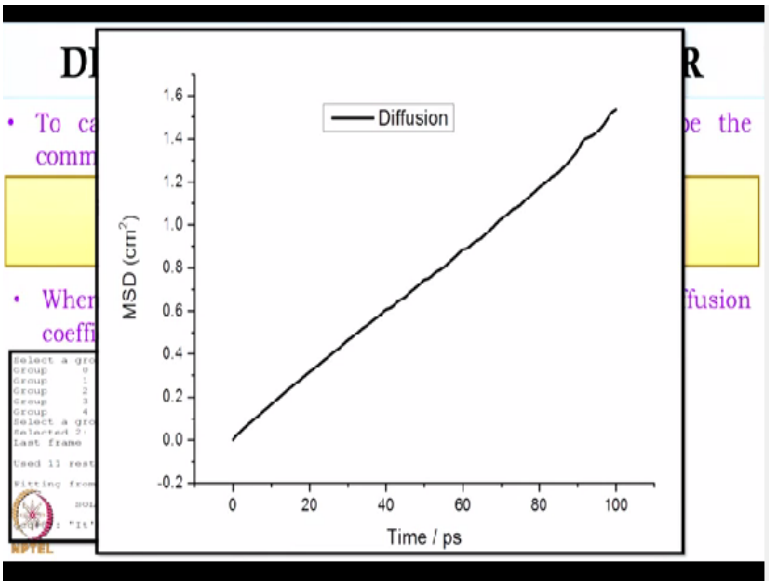

Something like this will be displayed which passes through the origin. So if they want to calculate the msd, they can calculate the slope of this? Yes. And you will get the same value. Same value. In the printer. Yes, exactly. Okay. So we will conclude this lecture. It was a little hurried at the end. It is okay. We will actually demonstrate it using the gromacs. So next time, we will consider something about the mixtures. So we will conclude here and see you next time. Thank you.