Computational Chemistry & Classical Molecular Dynamics
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Lecture – 35
Molecular Dynamics using Gromacs-3: Installing Gromacs

Hello again, so, so far what we have done is to get an energy minimised configuration for liquid argon is that the em.gro file, yes, yeah, so please continue, so we will now use the em.gro file that is the energy minimised configuration to run a full molecular dynamics simulation, so that we can get the trajectory file out of it,

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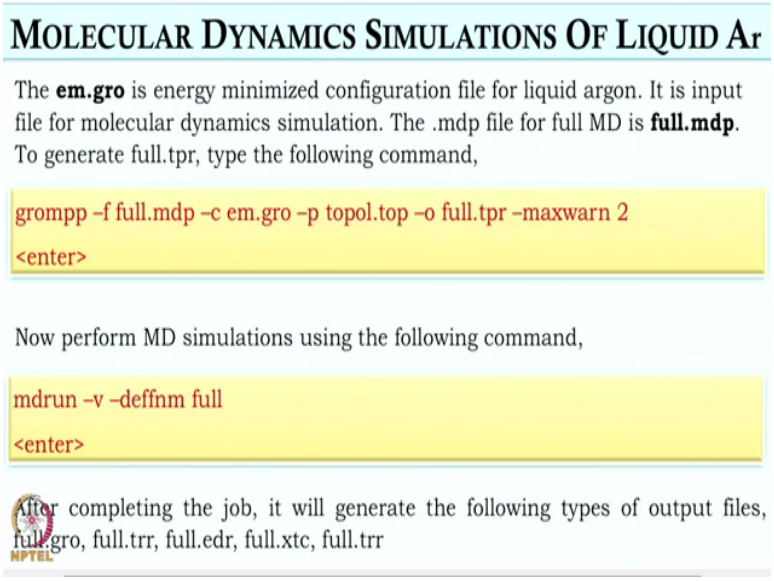

So, will again generate the tpr file using the command grompp, so we will type grompp –f full.mdp, which is the molecular dynamics parameter file for the full molecular dynamics simulation, then –c em.gro; em.gro is the energy minimised configuration for liquid argon then –p; topol.top that is same as before, yeah, that is the same as before and what are the differences in full.mdp and em.mdp?

In em.mdp, we are not specified that whether we need to give the temperature or pressure constant or not, we are not specifying that after how many steps we are going to save the trajectory file or the coordinate or the velocities, what is the way by which we are generating the velocities or in case of; so for energy minimisation, we do not need any velocity, yeah, we do not

need them, we are even not; in case of poly atomic molecules , we will be using algorithm to fix the bond length and bond angle, correct.

So, all these parameters we are; will be using in the full.mdp and not in the energy, em.mdp file, okay and then we will get a output file –o full.tpr –max1 space 2, so here the output file we are getting is full.tpr and now, we will run this full.tpr using the command mdrun to get the trajectory, so again when you say defn; deffnm that means all of them will have the same initial full and then we will get files full.gro which will be the gro file after full MD simulation.

Then, full. Trr, full.edr, full.xtc, so all have been; so instead of full, it can be any other name also, no, but then you have to have the tpr file in that name because since we; the tpr file that is the output file of grompp is full.tpr, okay, so we are giving –deffnm space full, if you give the em.tpr, you have to use em or if you give there grompp.tpr, you have to use grompp instead of full.

So, that 2 names have to be similar, okay, so now since we have all the trajectory file, so this whole information is contained in the tpr file, yes and I can view it what is the command to view? Gmxdump, so I can dump and view the full tpr file, yes but this is usually a very large file, yeah this is; this contain all the information in the gro file, top file and mdp file, now in fact I would recommend to all users that once in a while check the sizes from the files.

Because if the files are too much, I think it can; can it not fill the whole hard disk, yeah it cannot fill the whole hard disk, it depend on the size of the system, correct, suppose you have a file, , you create a box, which have 1 million atoms then it will have a large tpr file, so it is a good idea, every now and then to take all the files from the computer disk and to put on a separate external hard disk, yeah.

Because, otherwise the first time we run the program, the student gave 50 million step became you wanted to do a very large simulation, then the whole hard disk was full and then we have to call the expert to really restart the whole thing, so be careful about the file sizes and keep monitoring it; monitoring all the time, yeah, proceed, so after you get the full.xtc tpr and all file, so now we will analyse it trajectory that is we will calculate some properties.

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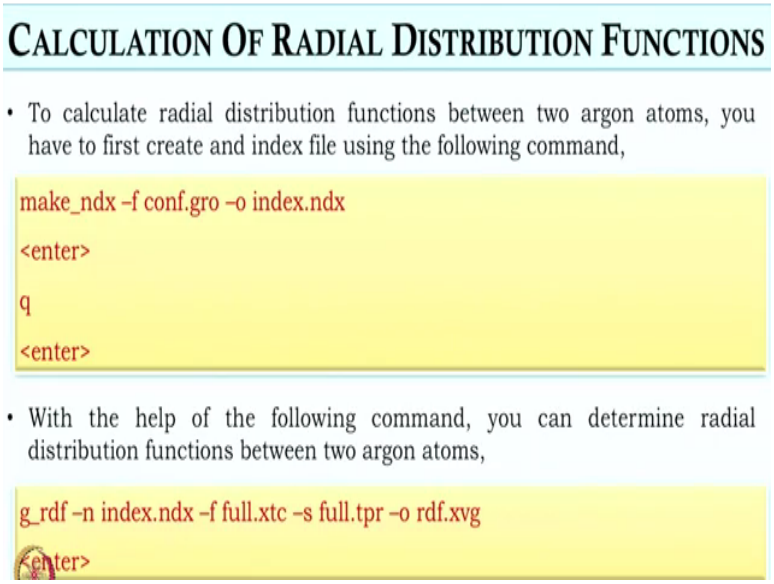

So, whatever the present simulation were done, were they npt or nvt; they were npt, okay since the constant number, constant pressure, constant temperature, okay, so we will first calculate the radial distribution function between 2 argon atoms, so to calculate we have to first, so what are the different types of analysis available; one is your radial distribution function, then you can calculate diffusion coefficient, correct, you can calculate the distribution of bond angle, dihedral angle.

Then you can calculate the spatial density map, then you can calculate the angular distribution function, different types of correlation function, hydrogen bond, so is there a list of all the analysis I can do, yeah, yeah, there is; when you install Gromacs, it will have a bin folder and in that bin folder, you will have a detailed list of command which are the command that is for analysis, okay, all the commands are given, okay starting from creating a topology file that is pdb 2 gmx to all the commands.

So, once you have the hydrogen bonded molecules, you can calculate the hydrogen bond lengths, yeah, bond lengths, hydrogen bond distribution, yeah, the energy of hydrogen bond, okay, correlation function involved in them, so can you calculate the say, average energy between 2 specific groups during the simulation, yeah, then you have to create 2 specific group using this

index, you have to create an index file for specifying those 2 specific groups between which you want to calculate the interaction or hydrogen bond.

So, suppose you want just the columbic interaction between 2 objects as a function, then you have to specified at between which 2 object you want the columbic interaction that you have to specify in the mdp file, in full.mdp, you have to type an extra line energy groups, so lot of options are there, what we can do on the website, we can give a list of all the things that can do and may be even store a set of results so that people can use it and test their skill, yeah, okay.

So, to calculate radial distribution function between 2 argon atoms, we need to first create an index file, so we can create an index file using the command make _ ndx, so what we need as a input here is just the gro file, so make _ndx – f conf.gro –o, which is the output file, index.ndx, then we type enter, then we have to type q; q is 7 exit and then again enter, so it will create an index file.

Can you view this index file using vi? Yeah, we can view this index file using vi command, okay, so now calculate the radial distribution function, we have to type the command g _rdf; rdf is radial distribution function space –n index.ndx space -f full.xtc; xtc is the trajectory file then space –s full. Tpr then space –o; o is the output file, rdf.xvg, so whenever we want to analyse any file or we want to calculate any property there are 3 files that is needed.

The first is the ndx file that is the index.ndx, then is the xtc file that is the trajectory file and then you say tpr file, these are the 3 file that is required for any kind of calculation, any kind of analysis, tpr file does not include some information of trajectory? No, tpr file does include; tpr include the information about the topology file, about the gro file and about the mdp file but it does not include any information regarding the trajectory.

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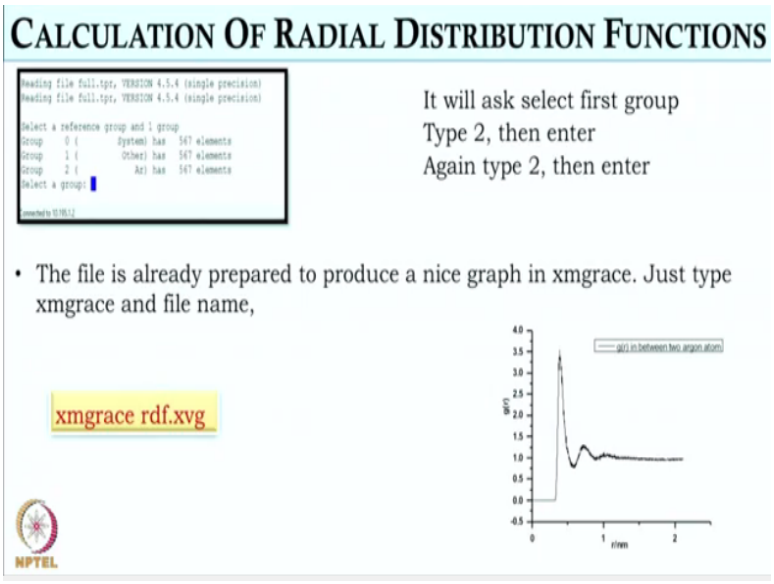

All information regarding trajectory is contained in the xtc file, okay, so there is a command, so after we type this command, it will ask us to select a group, so first we have to type 2 and then enter, so it will show something like this that select a group, so you type 2 and then type enter and then again you type 2 because it is between 2 atoms; radial distribution function, so you have to select 2 groups.

And then, the files is created it as rdf.xvg and then if; no, no the radial distribution function is between pair of atoms, yeah, right, so do not you have to give pair there? Yeah, so it will take first, it will take, when we type 2, it will take argon atom and then again, if we type 2, then it will again take the second argon atom, so it will calculate between 2 argon atoms but there I have seen 1 and 2 know, on the left; 1 and 2; see in that file, yeah, there is 0, 1,2; yeah, 0, 1, 2 since it is some mono atomic molecule and it just same molecule.

So, it does not matter 0 system, you can as well select 00 or 01 or 02 because all of them contain argon atom only but when we will have poly atomic or tri atomic system like water or CO2 there, we will have 3 different side, so we have to create index file for; in case of water say for oxygen, then for, there are 2 hydrogen, so we have to create an index file for 2 different hydrogen.

So, instead of 1, 2, can I give 1, 3 but there is no 3 in this case, so you cannot give 1, 3 because it is 0, 1 and 2, right, so you can either give 00, 01, 02, 11, 10, 12 or 20, 21, 22 because everything

is same here because it is a mono atomic molecule, okay but in case of triatomic or polyatomic molecule, we have to specify between which atom, like we have to create an index file for each of them, yeah.

So, rdf.xvg file is created, so when you give in that xvg file, it is a correlation function between argon atoms, yeah it is, does it average over all the 547, yeah it is average over all that 567 or 547; 567, okay, so, now we will display the graph in xmgrace, so an xmgrace is a plotting software, it is also free software, so we just type xmgrace rdf.xvg, it will display this graph between argon atoms.

This is the radial distribution function plot, where the x-axis is the distance between 2 argon atoms in nanometre and y axis is the radial distribution function, so that xmgrace already knows what labels to give? Yeah, it will put the labels, in nanometre, yeah, yeah it will put the labels because that must be already contained in their xpg file know, yeah, in xpg file, it is written that something there is distance and then there is the value of radial distribution function.

So, xvg file can be edited, yeah it can be edited, after it is created, you can edit it, okay and then it will plotted accordingly in xmgrace. So, if you want to view actual numbers, you can go to their xvg file and see those numbers; you can go vi rdf.xvg, then you can open the file and then you can view the file. See for example, on the gfr, I see that there is a minimum around < 1 nanometre, right, so I think it is around say, 0.65 or something.

So, from the graph, you may not be able to read, so you go that xvg file, edit it and you will know exactly, what is the value of the minimum; were the minimum is or what is the values, okay. So, this rdf.xvg contains only information about rdf, yeah, okay, so what are the next things we have here?

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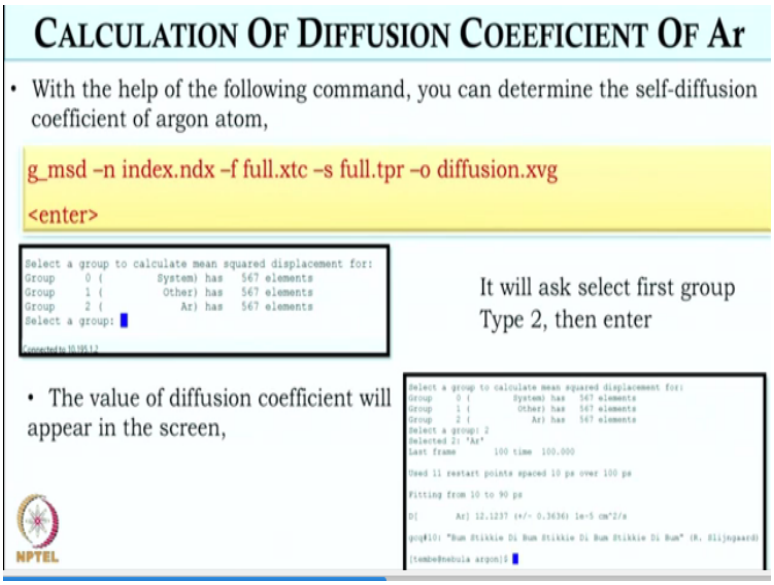

So, now if you want to calculate diffusion coefficient of argon atom, so with a type; with the help of this g_msd; msd is the mean square displacement, so you can calculate the diffusion coefficient of argon, so here also, we need 3 input file and the input file is same that is index.ndx full.xtc and full.tpr, then –o diffusion.xvg, okay, so if we just type it, here also again, it will ask to select a group, right for which atom of a which group we want to calculate the diffusion coefficient.

Since here 0,1, 2 all these 3 contain same information, so we will just type 2, so it could have been 011, no here we just have to type one group or one because we are calculating diffusion coefficient not between 2 atom and just one atom or one molecule in a diffusion. So, after we type 2, or 0 or 1, something like this will be displayed in the screen, so here we will have the value of diffusion coefficient as 12.2337 within bracket is an error bar.

And then into 10 raised to the power -5 centimetre square per second, so here it is being calculated using the Einstein's diffusion coefficient formula, we can as well calculate diffusion from velocity autocorrelation function also, now, suppose I wanted the plot of mean square displacement versus time, so you just type xmgrace, msd or diffusion.xvg, so it will a graph passing through the origin.

We will see it when we perform the simulation on screen here, okay, so now this is about the diffusion constant, yes, now since we have some time, why do not we just discuss the installation a little bit, sure, so installation usually you can do in about 15, 20 minutes, yeah if everything goes well, if something does not go well, are there some help sites were people can approach; yeah, there is Gromacs installation site, which is a free site where people do ask question about if they have difficulty in installation and all.

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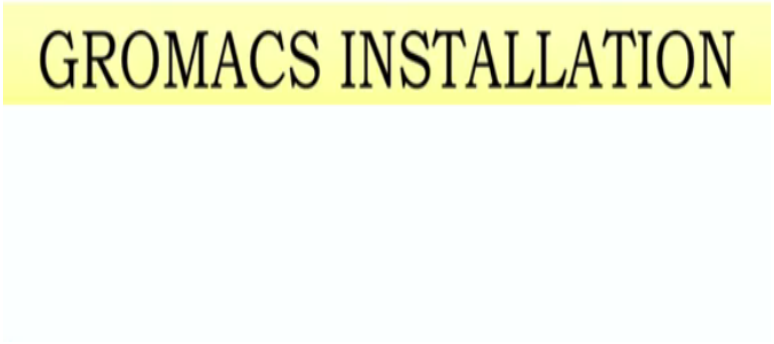

Can, you can always send a mail to us if you are stuck, students can send as a mail, sure, okay, so we will not discuss quickly Gromacs installation, they just the discussion, we will actually show the installation in 1 or 2 lectures, yeah.

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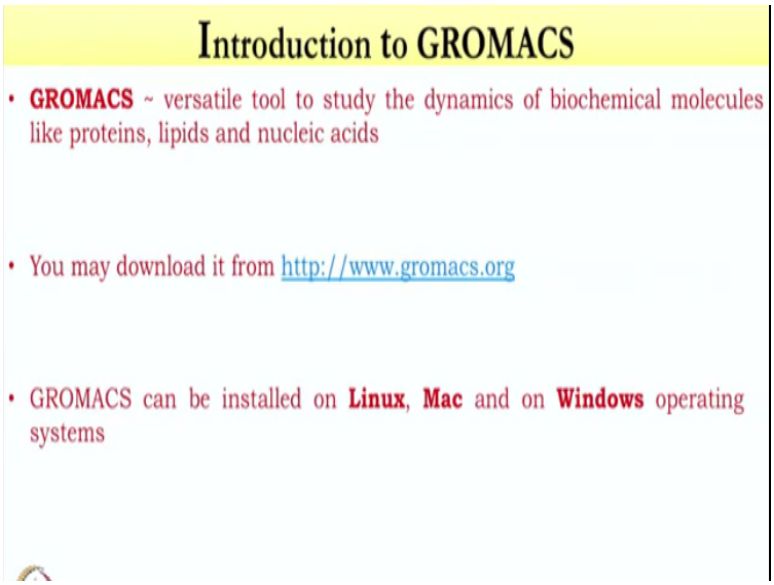

So, to install Gromacs, so Gromacs is basically, a free software which can be downloaded from the website given here Gromacs.org, so when you go there, there will be different version of Gromacs available, so download the latest version as a tar file.

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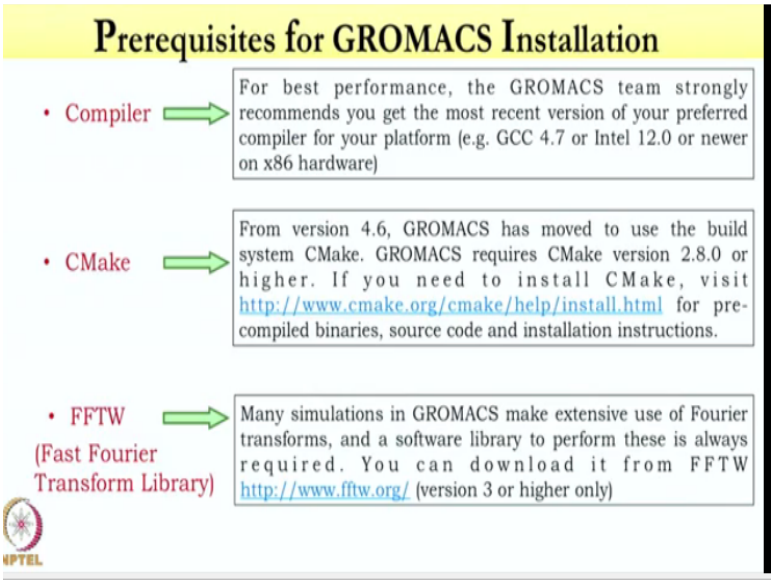

And to install Gromacs, no, no, go back, so that you can do that in windows also, yeah we can do it in windows also but windows is a paid software but Linux is free, right but what is the kind of minimum RAM that is needed roughly, suppose I have 4GB RAM, is that enough, 4 GB; I guess more than that is required because just installation is not enough, when you install it, you might as well want to perform simulation, correct and so there, the file will be very large in size.

So, I guess, minimum 8GB, yeah 8GB is fine, okay, so Linux is easiest because it is a free software and plus also I think in Linux, the entire memory will be available, yeah, so whereas in windows, the windows itself will take a new space, correct, okay, so to install Gromacs in your machine, there are 3 things that is acquired. So, first you have to have a compiler that is g++ compiler.

Then we have to have a Cmake and we have to have a FFTW also, so all these are free and it can be downloaded from the website link that is given in the slide.

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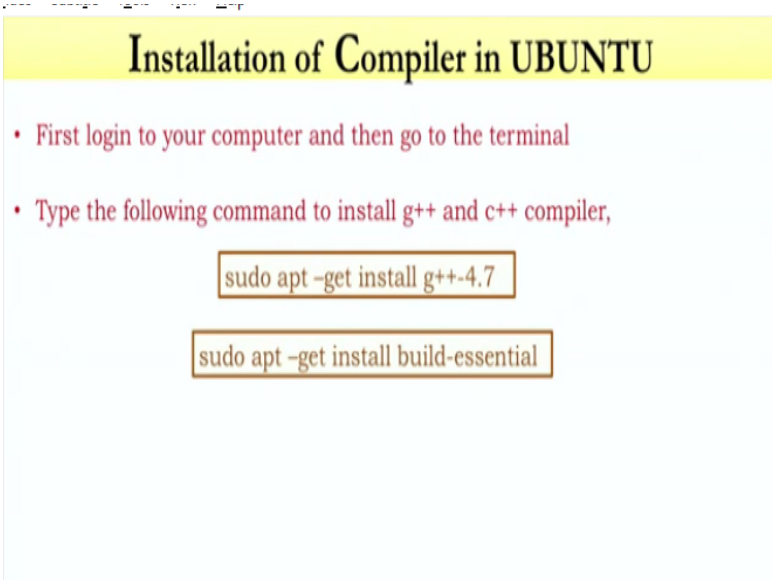

So, first we will have to install the compiler say in Ubuntu, so to install it just type the command sudo space apt – get space install g++ 4.7, it will automatically get installed in your PC, so after g++, is there a minus sign there, yeah -4.7, it is the version, okay, it is the latest version now. So, you have to type it; first you log into your remote machine and then you go to terminal in Ubuntu and then you just type sudo space apt –get space install space g++ -4.7.

So, what will this install; it will install the compiler g++, okay, so after this; but is it possible that Linus itself has a g++, yeah, it is possible that Linux; if it already has g++, it will just show that the latest version is already installed, okay, it will get the command but if you do it, will it reinstall on top of the old one or; yeah, it will reinstall, if an older version is installed, it will reinstall an updated version, okay.

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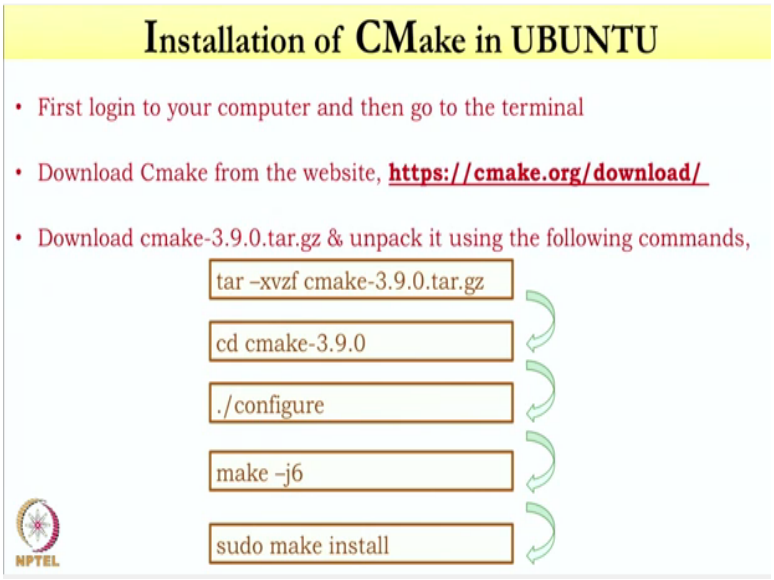

And the next one is what; next one it will just update all the software that is installed, okay, so now to install Cmake in Ubuntu, so first you have to download it from the Cmake.org, it is a free site, free software, you can download it the tar file and then you untar the tar file using tar space –xvzf space cmake whichever version is available but preferred is the latest version, okay, then you go to the directory cd space cmake.

Then, there will be a file contained; named configure, so you have to configure it using the command ./configure, after the configuration is successfully done, then you have to make; type the command make space -j6, so it will make the file and then sudo make install, it will install Cmake, so these are the 4 steps, so all these are just to install the Cmake, yeah and same command you have to install FFTW as well.

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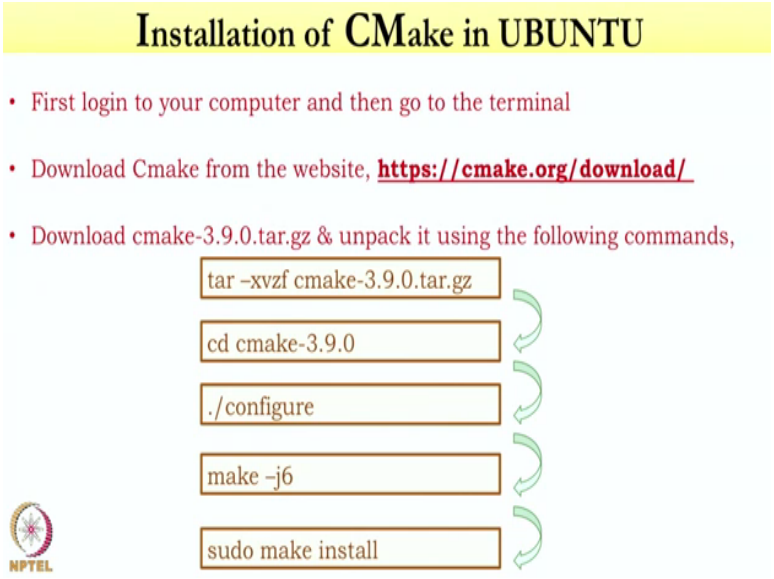

So, install FFTW from the site fftw.org, it is also free site and then you will download the tar file, and you have to untar it using the tar – xvzf command, then you go to the directory FFTW, then you configure it, then you may and then make install, so same as Cmake. So, in which directory does it install, so wherever you download the Cmake FTTW and Gromacs, all these 3 have to be in a same directory.

Suppose, it is in initially, when you download it, it will go in a download folder, okay, so you go to CD space download and then you first unpack Cmake, then you unpack FFTW there and then you install Gromacs in the same folder because all 3; Cmake, FFTW and Gromacs have to be in the same directory, okay, so what is the typical name that you want to give to that directory, it is user defined, okay, so what do you do; you just give Gromacs to the directory.

Yeah I just give the Gromacs as the directory, okay. So, then you install FFTW using this command, this is same as Cmake, okay

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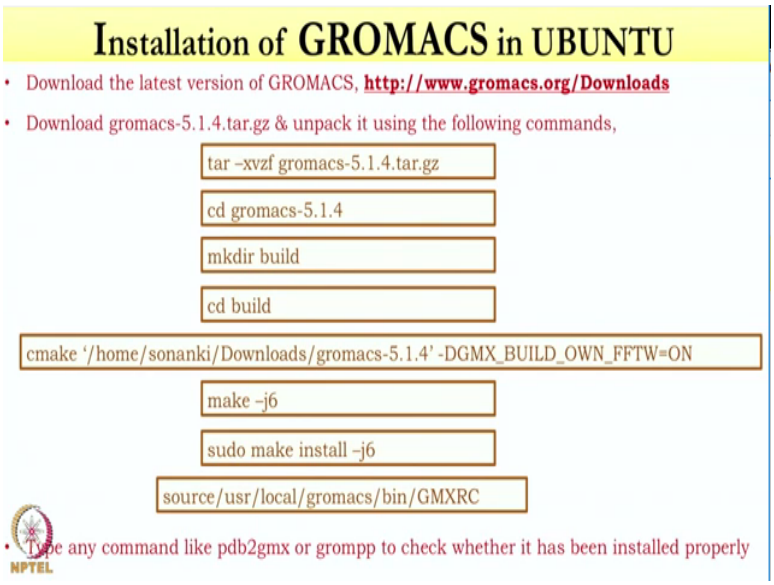

And then to install Gromacs, you will also have a tar file there, okay, so you just unpack it using the command tar space –xvzf space Gromacs, so what is this xvzf do? It untars the; unpacks the tar file, okay, then you go the directory using CD space Gromacs, then you have to create a directory named build but have we created Gromacs directory to begin with?

No, we have not created, we can create CD Gromacs and then we can have all these 3 files in the Gromacs directory and then we can one by one start an installing, okay, right, so then you have to create a directory called build, so typing the command, mkdir, so when you; so this build will be a sub directory of Gromacs, yeah, it will be a sub directory of Gromacs, then you go the directory CD build and then you have to type the command, cmake space.

And then wherever your Gromacs is install; downloaded, you will just drag the folder, it will automatically give the path, so that Gromacs - 5.1.4, is it a untared file already, yeah it is a folder, okay, so so wherever it is downloaded, so you just have to drag the folder there, it will automatically give the path supposing in my case, it was downloaded in home, then sonanki, then downloads and then there was the Gromacs entry.

So, this was the folder, okay, where it was downloaded and then you have to type space - all in caps; DGMX_BUILD_OWN_FFTW =ON, so after this it will be take 2 or 3 minutes to install Gromacs, then you have to type make space –j6 use and then sudo make install and after the

installation is done properly, you just type source, use a local Gromacs, bin GMXRC, so this bin directory, you will have all the commands, okay.

So, to ensure or make sure that Gromacs is installed properly or not, you can type any command to just check. If it is installed properly, it will give you a list of thing, like if you type grompp, it will write at okay, this is the input file option, this is the output file option but if it is not installed properly, it will show nothing, okay, it will say this is not installed here, please type other thing to view.

So, how many more things are there, is it complete now anymore or? Yeah, Gromacs installation is done, so it just take 10 to 15 minutes to install, so now if somebody asked a question, why I should spend these 15 minutes, what is your response? If you want to use Gromacs, you have to spend this 15 minutes and it is very free software, it is fast, you can simulate large number of molecules.

What I would like to say is that, you can calculate all the equilibrium and dynamic properties of liquids and mixtures and ionic solutions, yes, literally you can do most of thermodynamics and a large part of kinetics in solution media, yes except the chemical reactions, yeah, okay, so for example, people learn about free energy, people learn about entropy, these are all objects which we hear and we do not have what the actual values of for a given system.

See for example, we want to do simulation on water, so I want to calculate; let us say I want to calculate the heat capacity of water, yeah, can I use Gromacs to do that yeah, we can calculate heat capacity using Gromacs, okay, so the way I would do heat capacity is the rate of change of energy with temperature, yes, correct. So, what I would do? Suppose, I want heat capacity at 298 kelvin, yeah, so I would calculate the average energy of the system at 298 and energy at say 296, then 300.

So, as the function of temperature; if the energy as the function of temperature, I can take the derivative and get heat capacity, so I can get heat capacity at constant pressure as well as heat capacity at constant volume because cv and cp are different, yeah, so I can do simulation at

constant volume which is nvt to get cv, yeah, I can do at constant pressure which is npt, so I can do this, okay.

So, for example, now, we want to know, let us say the average number of hydrogen bonds between each water molecule in a liquid, so how would you do that? G_H bond, okay so that is part of your list of; list of commands, yeah, okay, it calculates and it uses the geometric definition which is already installed, it will take the minimum distance angle criteria to calculate. So, now suppose, I want to change those parameters; so, you specify the bond angle and you specify the bond length, you can do that as well.

So, if the software has its own definition, I can give a different definition; you can give a different definition of your own choice. Suppose, I have O HO bond typically, we take 30 degrees, yeah as the bond angle, yes, but I want to give it 40 degree is to see whether, yeah, you can use it, right, you can change it, okay. So, to summarise what we have done so far, what we did was we gave all the files that were needed in the Gromacs software, okay.

And gave 2 examples of execution; one was to calculate the pair distribution function and another was to calculate the diffusion constant of course, we did not plot the curve for diffusion constant but that is very easy using your xmgrace and we will show it; so then we gave basic installation commands in Gromacs, so you have already see the commands, after 1 or 2 lectures, where we consider water and one mixture, so let us see what these command are.

And once we are familiar with the commands, we will start the installation procedure, so that you when we start installing, then you already know what commands that have gone into that and you will get a much better feel, so that we will do after 1 or 2 lectures. Today, we just conclude here, where we have the one basic command for installation and are there some manuals where these are available.

Yeah, for each version of Gromacs, there are manual available and it can be downloaded, it is free of cost, so okay one good idea would be whatever we are giving here in a few lecture is a very small subset of the whole thing that is available, so I would recommend to the users just

start reading the manual because in many of these manual, lot of theories also given, right, each algorithm is described in detail.

When we discussed specific algorithm, for example what is that ewald some, what is the particle mesh ewald, what are all these potentials, what are all these parameters, so it is a good idea to look at the manual as well, so when we do some actual calculation and do the analysis, it will also tell you what these things mean but it will give you; it is an investment and whatever work you do in the future, all of thermodynamics and kinetics will be actually possible to verify this in by yourself.

So that is the great advantage of this very powerful, so if you know how to use Scilab well and how to use Gromacs very well, there are many things what you learnt in school or college, you can actually verify in your calculations. So, we will conclude this lecture here and continue with water next time, what you want to do; yeah, water and mixture, simulating water and simulating the mixture that is what we will do in next time, so we will conclude here, thank you.