Computational Chemistry & Classical Molecular Dynamics
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Lecture – 39
Molecular Dynamics using Gromacs-7: Gromacs Installation (Continued)

So now we will start the procedure for installation of gromacs. Remember we have been using all these programs for demonstration. Now we want to start at the very beginning when we start installing gromacs from the website, okay. Please show the website from where, show the website, yes.

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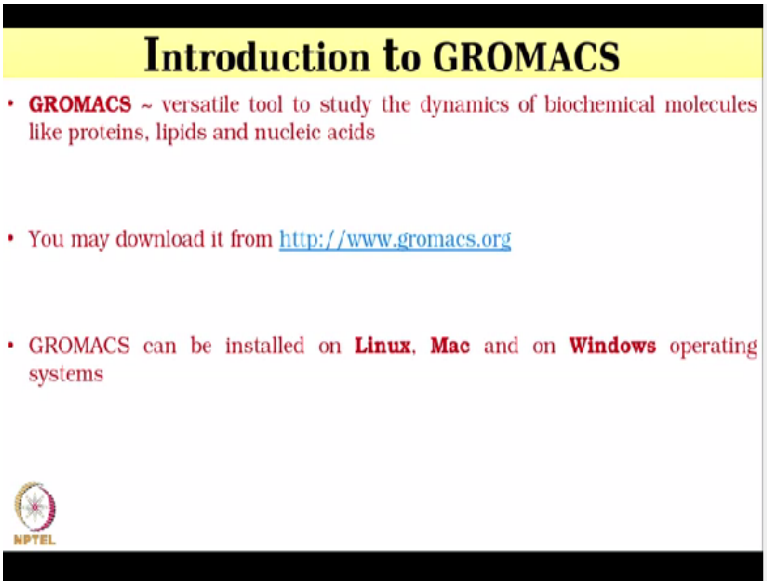

This is the website www.gromacs.org where the software gromacs is available free of cost from version 3.1 to the latest version 5.1.4 is available and any user can download it.

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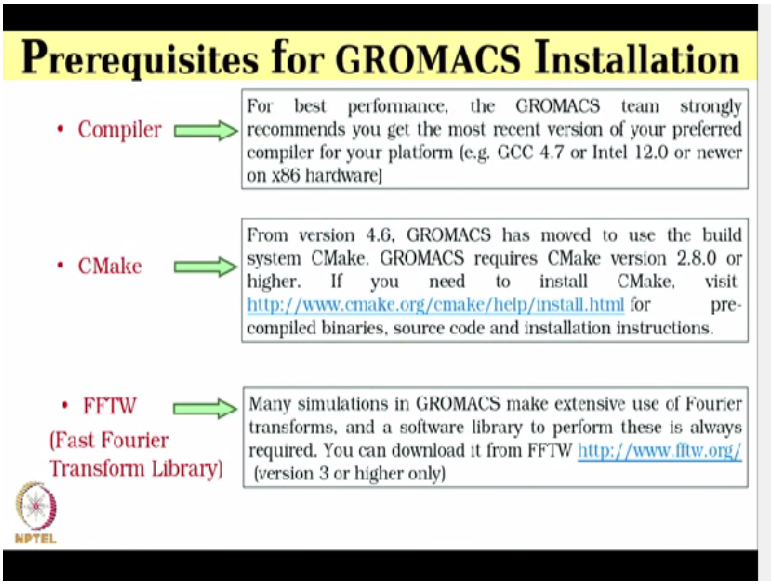

And for successful installation of gromacs, you also require a compiler, CMake and FFTW. So compiler can be installed in Ubuntu free of cost and in some cases, it is already preinstalled. Preferred one is g++4.7. One also needs CMake for successful installation of gromacs and CMake should be higher version from version 3.1 and it is also available free of cost and one can download it from the site www.cmake.org.

Similarly, one has to download Fast Fourier Transform Library that is FFTW for gromacs installation. This is also available free of cost in fftw.org website. And version 3 or higher is preferred. So FFTW, they are using for calculation of Coulomb potential. Yes. Okay. Exactly. So now I have already downloaded gromacs, CMake and FFTW in my machine and now I will show the installation step by step.

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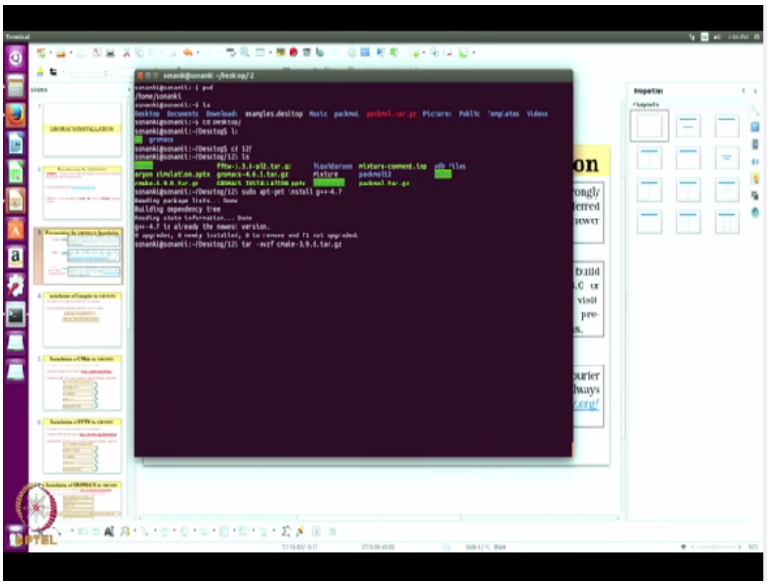

So I will just go to the terminal. So this is my terminal and this is my home page. If I just type pwd, it will show me the path. So this path that is home and my name. So now I will just type ls to display all my directories. So I will go to desktop and in desktop, I have 2 folders, 12 and gromacs. So in 12, I have all the files I have downloaded here. So there we can see that there is fftw, there is cmake, there is gromacs and also there is packmol.tar file.

So after successful installation of gromacs, we will also begin with the simulation. So now to install gromacs, we will need compiler. So to install g++compiler, we have to type the command sudo apt-get install g++-4.7. 4.7 is the version. Version, okay. So when you type it, it will already show 0 upgraded, 0 installed. Since it is already installed in the machine, so it displays like this. If it is not installed, it will ask for the machine's password to install it.

So if you want to uninstall this, what do you do? You have to go to program files and then uninstall it from there. Okay. You cannot uninstall from this directory? No. Okay. So since g++ is already installed, now so first we will start installation of CMake. So since it is a tar file, first we will untar it using the command tar-xvzf, then cmake.

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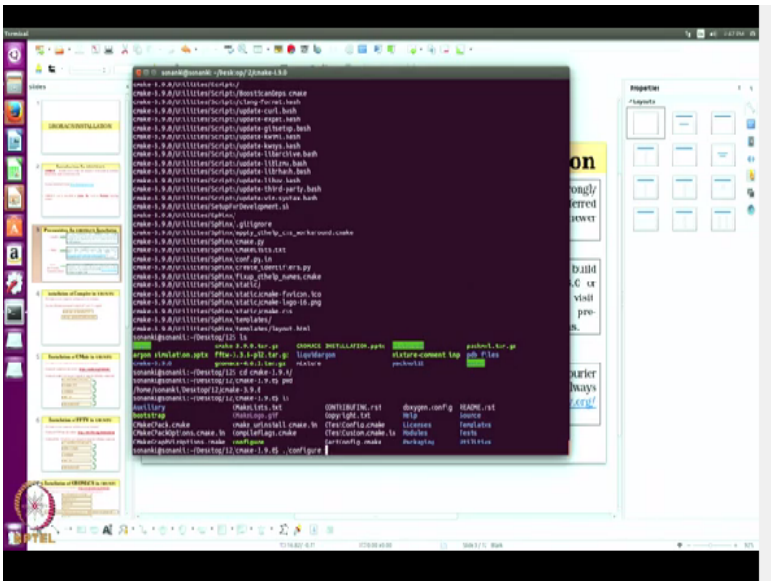

So it will first untar the file and now we will go to the directory. So if you type ls, we will just see that there is a folder created cmake 3.9.0. And now we will go to that directory. cd cmake-3.9.0. Can you do a pwd so that they know which is the full path? Yes. Pwd, it will come home. Okay. Then the name of my machine and then desktop. Since I am doing all my work in desktop, I mean in desktop I have made the directory 12 inside which I am doing all this. Right.

So 12 and then cmake since I have just untarred it. Yes. And now if you type ls, then we have file called configure. So now you have to configure cmake.

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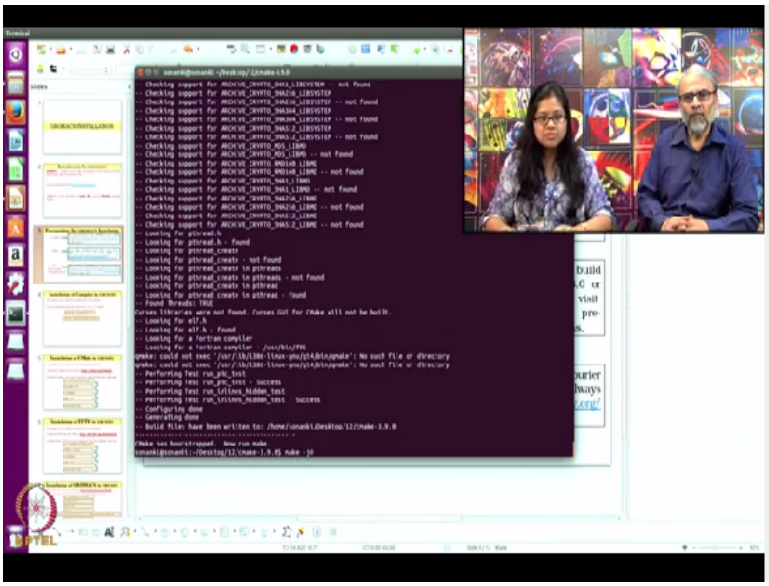

So to configure it, I will just type ./configure. Now it will start configuring cmake. How long

does it take? Not too long. No it just takes 1, 1 minute, 1 or 2 minutes. So after this, can you do that ls -l so that we will see all the executable files it has created? Yes, sure. Okay. So what is it doing now, right now. It is configuring cmake so that it can be used. Okay. So cmake you will need it for all the other installations also?

Yes. Okay. So cmake seems to be something like a compiler? Yes, kind of. Right, like when you do gfortran. Yes. It is compiling the text file into a executable file. Executable file. So cmake will make executable files out of all these FFTW. Yes. And you have g++. Yes. You need cmake even for that packmol? No for packmol, we need gfortran. But suppose the machine does not have gfortran, can you download it?

Yes. It is easier. I will just show when I install packmol. Okay. I will first install gfortran. Okay. Because in Ubuntu or Linux, gfortran is already installed in the machine. Okay. And if you want to install it, it will install. It will ask for upgradation if required. Okay. So what is the present version? Present version I have to check what is the present version. When I installed packmol, I will just check.

And is there a way to get which version if installed, are there some commands? Yes, there might be some Linux command to check which version is installed. Okay. You just have to type cmake, then --version. Then it will display which version. Okay. Is installed. And installing all these files from the net, it does not rather download it. It takes hardly 5 minutes or may be less? Less than that.

Less, okay. Because the folder is like 4 to 5 MB. Only the gromacs folder is around 10 MB in size. Okay. But FFTW and CMake is 4 to 5 MB. Okay. So total thing is hardly about 25 MB. Yes. But usually when we do this a.out in fortran. Yes. The a. files are fairly large in size. Yes, because that contains result and all. Even in gromacs, when we perform simulation. Okay. It depends on the number of steps and after how many steps are you saving your trajectory and all.

Okay. Depending on that, your output file size becomes sufficiently; The output file will be controlled by how many steps you are doing. Yes. That is. Right. Controlled by user. But when

we compile in Fortran, most of the a.out's are similar in size because program, number of lines in a program that user writes is hardly about 100 200. Yes. 300. Okay. Has it finished now? Yes, the configuration is done. Now we have to run make command to successfully install it. So I will just type make -j6.

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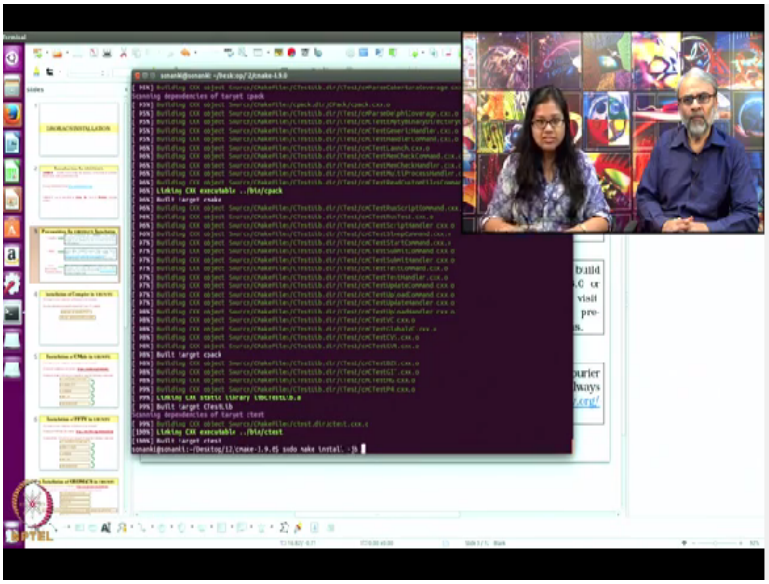

So now it is making all the files which are required for CMake. So what is the need for this particular command? Because it will, after this command, we will install it using make install. Okay. So I have just configured CMake. Okay. Now I have to install it also. So this is the installation of CMake. Yes. There is 1 more step involved. What is that? That is sudo make install.

Okay. So it will install it. That is the final step? Yes. That is the final step. There are 4 steps. First you have to untar it. Okay. Then you have to configure it. Right. Then you have to install it. Okay. But 3 steps? Yes. Like installation required 2 steps, make and make install. Okay. So basically there are 4 steps. So in which directory is it going to do this now. The same directory where I have downloaded, wherever I will download it or wherever I will untar the file.

Okay. It will be saved in that same directory. Okay. So suppose you are in directory X? Yes. And there is a file and you untar that file in directory X. Yes. Where will the files go? In directory X because I am untarring it. So whenever you untar, it remains in X only. Yes. Okay. But then you

end up having so many files in the directory? Yes, there will be bin file, shares, script, shell. Right.

So is there a way to have a more compact arrangement in your files because whenever you do ls in that particular. Because. Directory, suppose there are 50 or 100 files, it becomes difficult to locate them know? Because whenever all the softwares are installed, they were by default created files. Correct. So we do not have control over them. So now I think this is done. Yes. Now I have to just run sudo make install for the installation. So I will type sudo space make space install space -j6.

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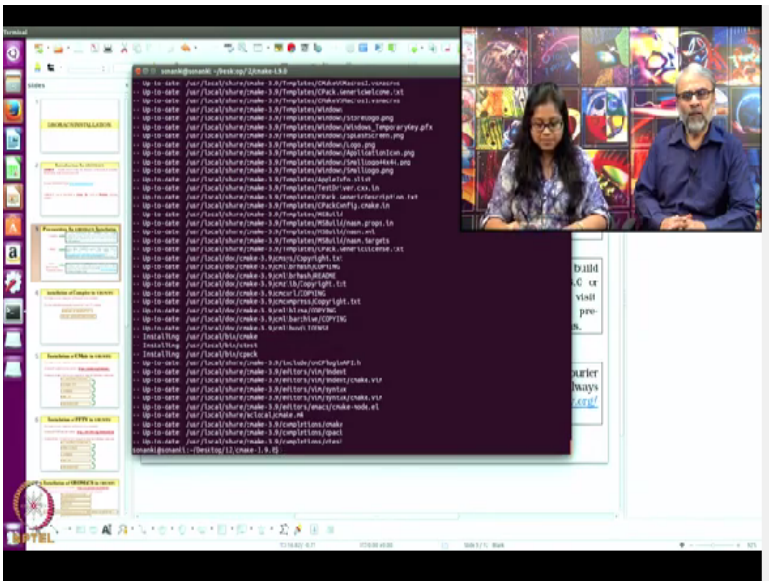

So it will install it. So this is installation. And my installation is complete. Okay.

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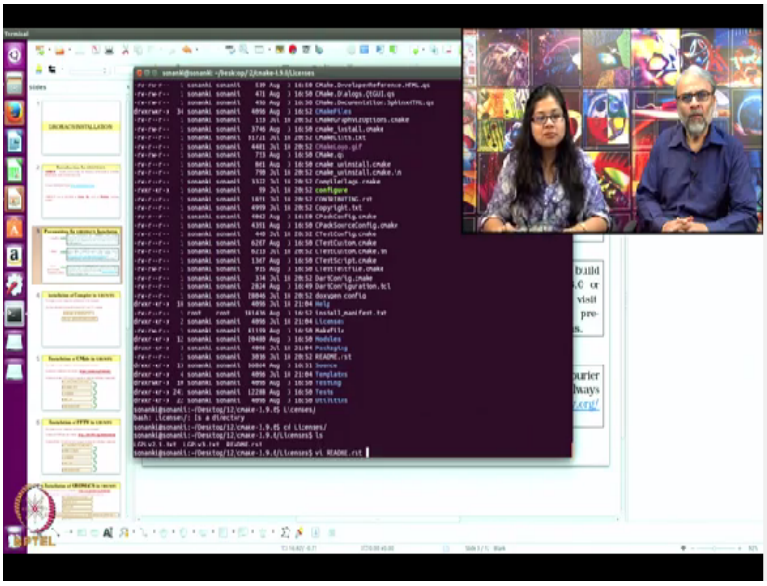

So can you do ls -l. Yes. So this is ls -l. Okay. Now, okay. So see many of the blue coloured things, they are executable files? Yes. Like help is an executable file. Right. What is that the one below help? Licence. Okay. So just type licence and see what it does? It is a directory. Okay. So I guess there will some.

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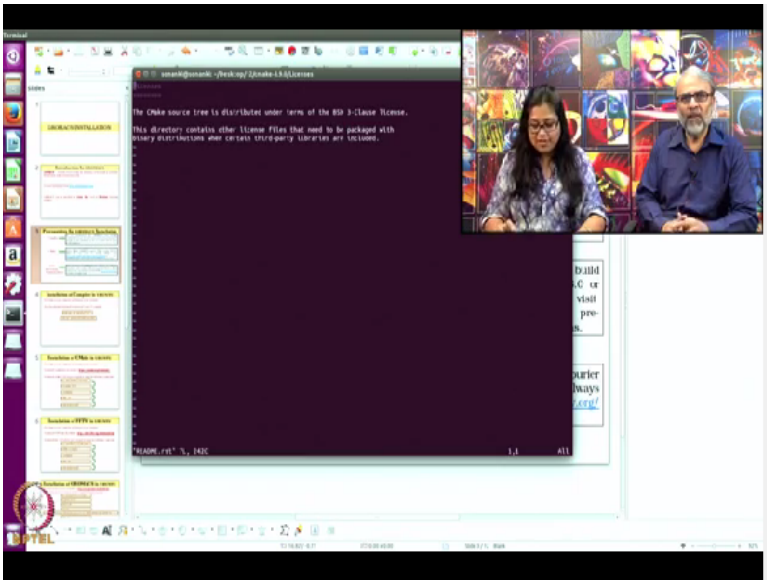

Okay, just some information. Yes. Okay, we can go back. So after CMake is installed, we will proceed towards the installation of FFTW. Okay.

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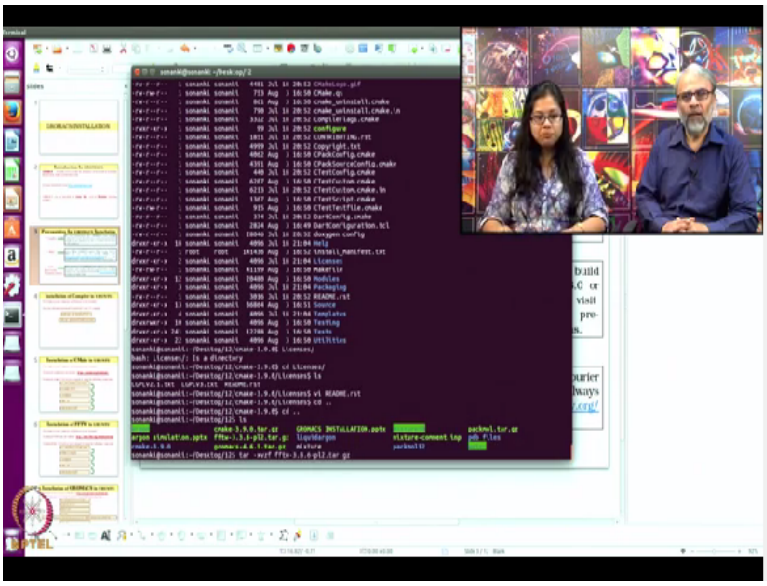

So for FFTW also, we have tar file. Okay. So first we will untar the file using; Which directory is it now. It is the same directory, in desktop, in 12, I have downloaded all this file. Right. And the same directory I have installed CMake. Okay. In the same directory I will be installing FFTW and gromacs. Okay. So to install FFTW, I will first untar the file. Okay. Using the command tar. Okay. Space -xvzf. Okay. Then space FFTW, the tar file name. Okay.

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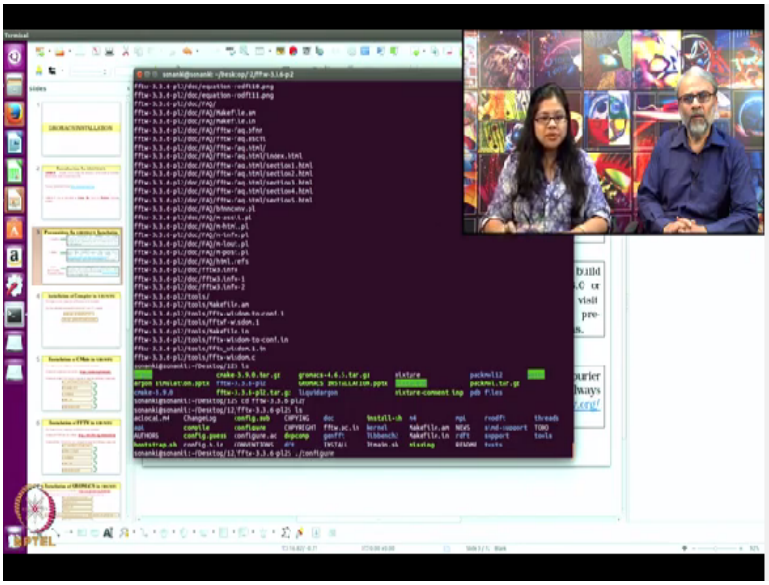

So when you type it, it is untarred now. Okay. Then I will go to the directory. After untarring, it will create a directory FFTW 3.3.6.PL2. Okay. Right, so now I will go to the directory using the command CD. Okay. So CD FFTW. Okay. And similarly we will have a file configure here also. So we have to configure it using the command .. /configure Okay.

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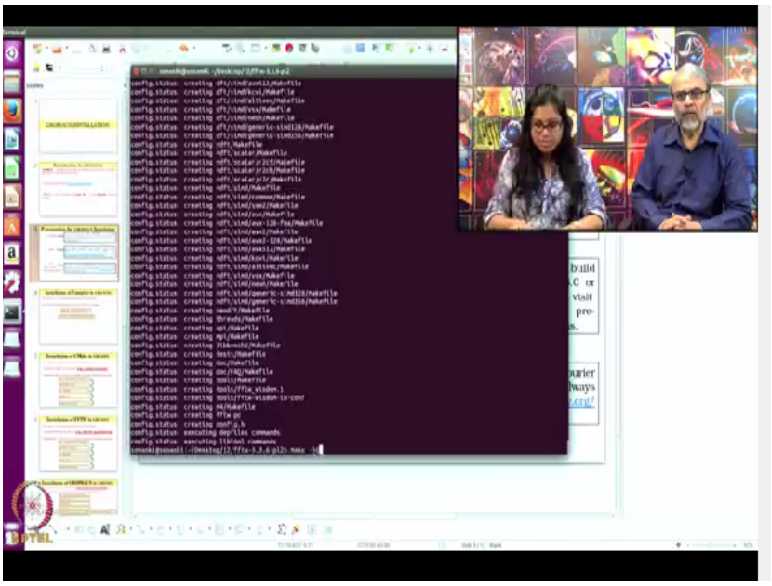

Same procedure as CMake. So this configure command knows what to do? Yes. You do not have to give an input or; No, It is all default. Yes. For your earlier one, which was the one before FFTW. CMake. In case of. There also you had to configure. ./configure. Just configure. Yes. So configuration is done. I will go to make. Okay. So make -j6. Yes.

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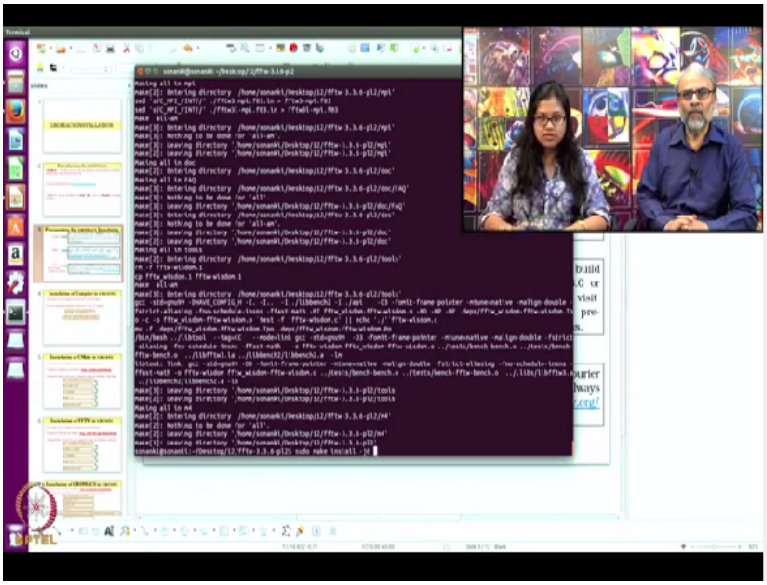

So it will make all the files required. And after that you have to do again make install? Sudo make install. Okay. So it will install it successfully. Can you tell what is the sudo command? Sudo is for super user, like since it is an administrative. Correct. Thing that I am using. So it requires password for your machine. Okay. So now I will do the installation using sudo make

install -j6.

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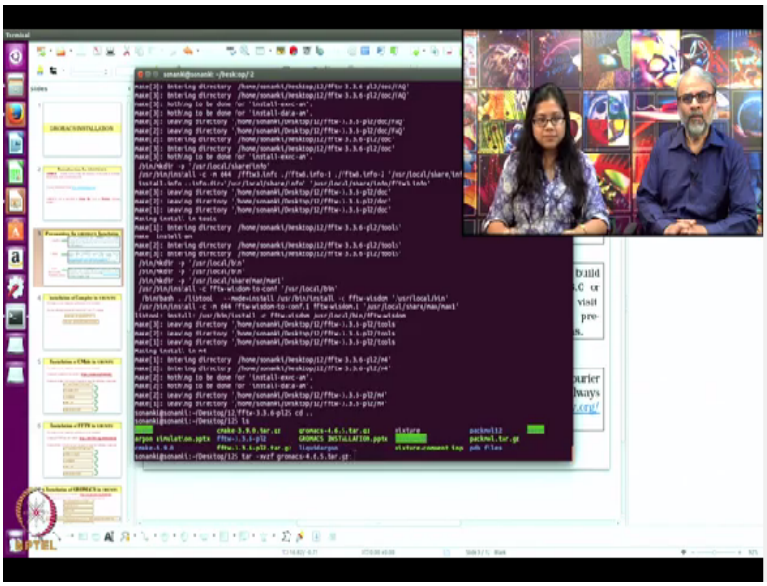

What is that j6? It is just given. If you do not give it also, it does not matter. Okay. So FFTW is also successfully installed. Okay. So now I will install gromacs. So I have gromacs 4.6.5. So here also I have that tar file. So first I will untar it using the command tar. Okay. Space -xvzf gromacs. Okay. So this takes probably a little longer or is it done? It is done. Okay.

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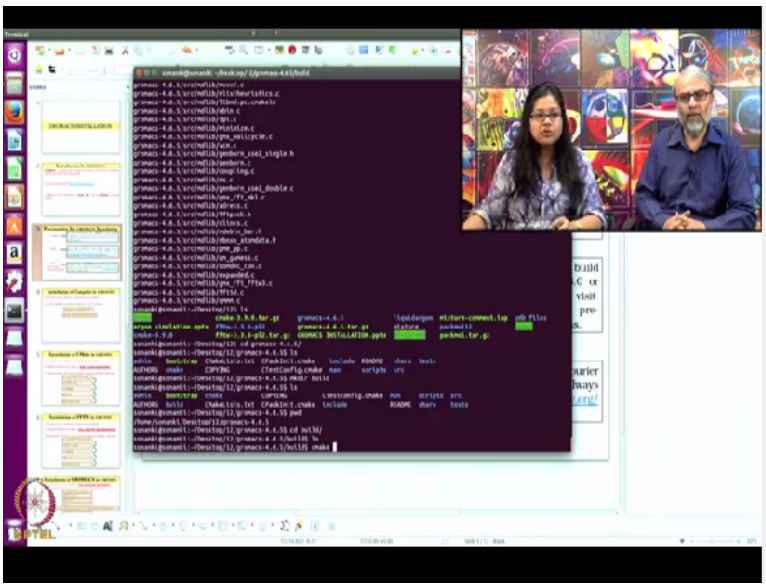

So now it will have a folder created gromacs 4.6.5. Okay. So I will go to the directory. Right. And then I will type ls. Okay. So now I have to create a folder build here. Okay. So mkdir build. So why do not you show the path again so that? Yes. So pwd. Right. So the path is home. Right.

Then my machine's name. Right. Then desktop. Okay. 12 and then gromacs. Okay.

So this is that. So in that you have created a build now. Yes. So you have to go to build? Yes, I have to go to build. So I will now go to build. Okay. So now here, I have to install, I have to now install gromacs. So for that I will first type CMake. Okay. And then I have to give the path where my gromacs directory is installed. Okay.

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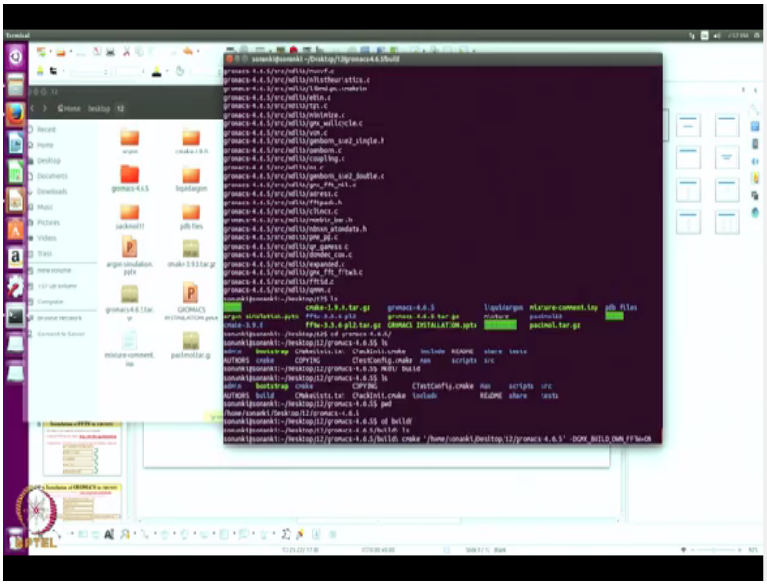

So the easiest way to give the path is, I just go to my files. Okay. Do you remember the path or no? Yes, but it is easy to just drag it. Okay. Because it automatically. It is your desktop on the left. Yes, this is my desktop and this is my folder 12. Right. Where I have downloaded all the files. Right.

So the one where gromacs is installed, the folder. Yes. So I will just drag it from there to here. Okay. So it will automatically give the path. Okay. You see. Yes. So I do not have to write anything. Much faster and no errors. Yes. Okay. So now I have to type some command that is -dgmx _build_own_FFTW =on. Okay.

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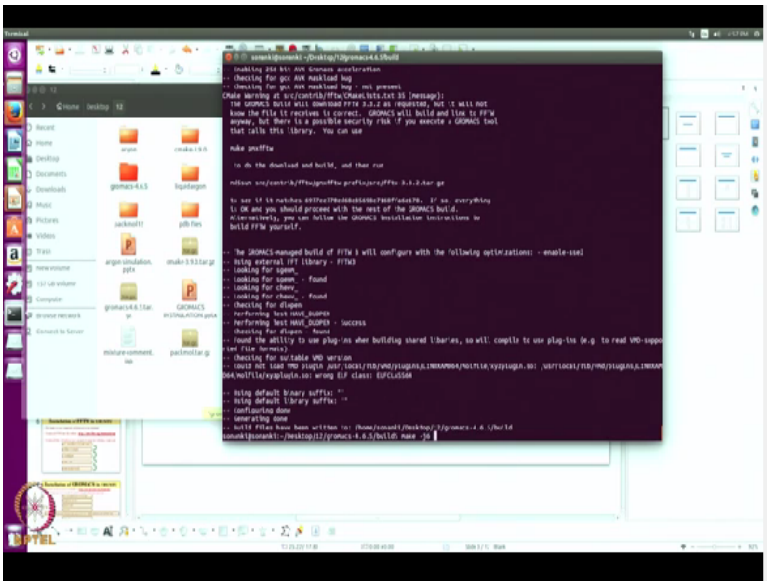

So what we can do later on, whatever commands are used, we will list all of them and put in a pdf file. Yes. So that it is easy for a new user to remember it. Yes, yes, sure. Okay. So now this is done. So configuring is done. Now we have to install it. Okay. So I have to type command make again. Okay. So make -j6.

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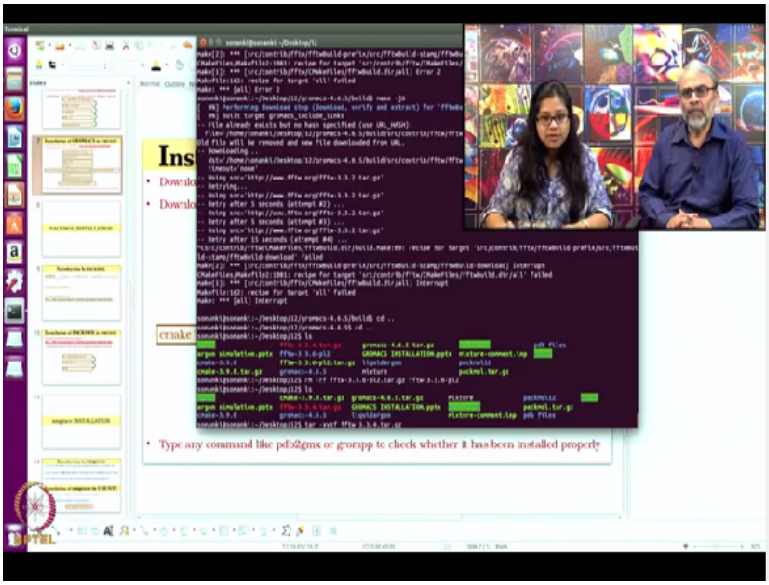

Is it doing? Yes, it is doing. It is downloading. Okay. So 0% and then it will show percentage. It will take some time. May be 1 or 2 minutes. Okay. So now you have typed make, this is for gromacs final installation. It is the same thing. I have just one extra line typed here that is CMake. Okay. And then I had given the path where my gromacs is installed and then I have typed build CMake FFTW own.

So that it tries all the, it is downloading everything. So suppose the path is not given, it will give some error? Yes, it will show some error. Or it will say please give the path where it is located. Yes, yes, definitely it will say that. Or there is some warnings or, no it is saying retry something. Yes. But all the files are already downloaded now. Yes. We do not need anything. No, no. I have already downloaded all the files.

Okay. Is it showing any percentage or it is saying retry? Retry after 60 seconds. Okay. So we have thus done this command and now we are doing make j6. Yes. Okay. So retry means do you have to type that again or? No, no it will just show it. By itself? Yes. Okay. So if some command is not working, how do you come out of that command. Some control Z. You just control C, then it will just stop your thing.

Right. So I will just come out of the folder. Yes. And it is showing some error in FFTW3.3.2tar.gz. Okay. So. So you will install FFTW again. Yes, I will install it again. Okay. 3.3.4. So I will just remove the previous version using the command rm. Okay. -rf. Yes. FFTW 3.3.6. This one .tar.gz and the file as well. So now I have uninstalled it. Right. And I will install again using the same command. First I will untar it using tar. Okay. Space -xv. So this is new FFTW? Yes. Okay. xvzf. Okay. FFTW.

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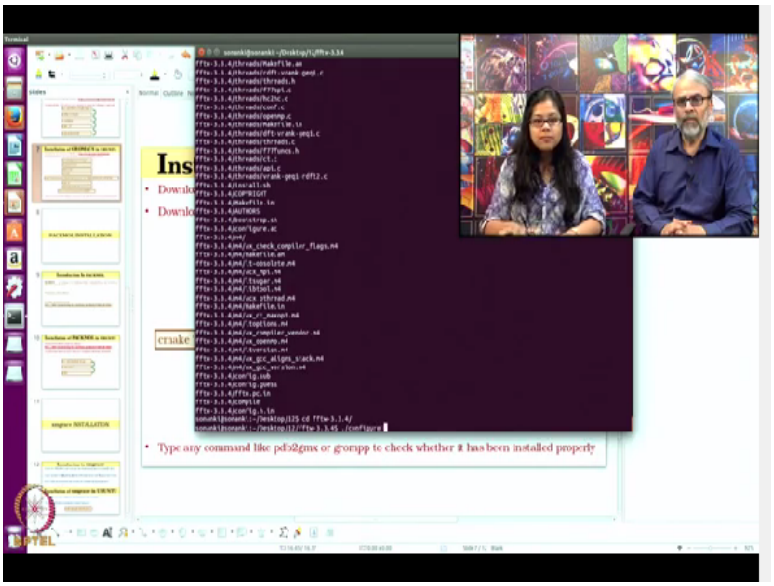

So untarring is done. And I will go to the folder. Yes. Which is created. Right. So here also first I will configure it using ./configure.

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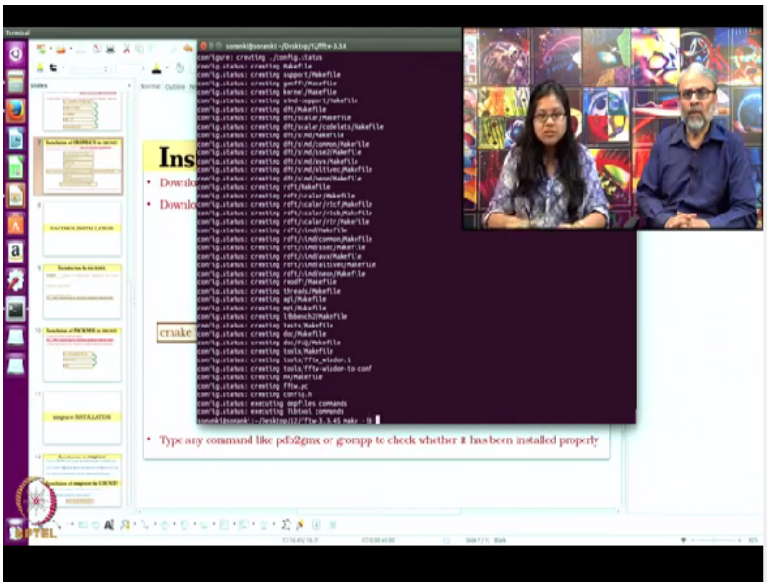

Was it the correct version of FFT3W. Yes, it was the correct version. Okay. So configuration is done. Now I will make -j6.

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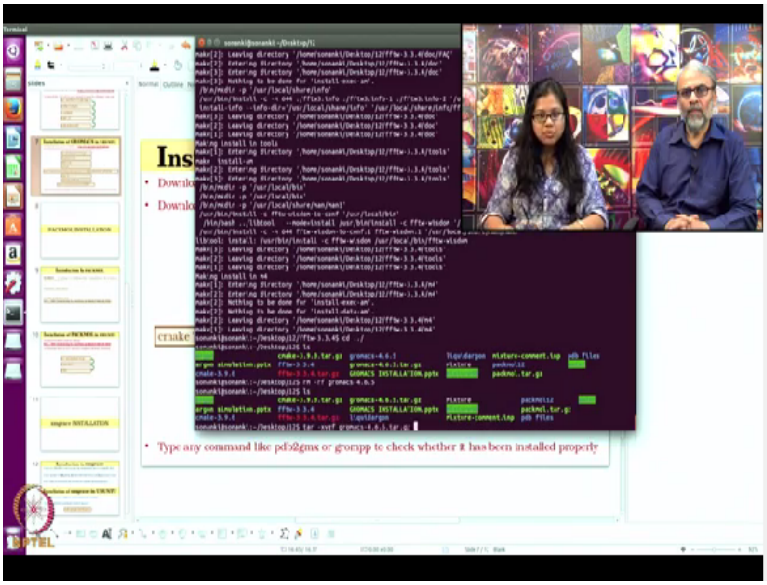

Okay. So it will make all the files. Okay. And then I will install it. But did it give an indication that there was a problem with FFTW? Yes, it was written in the word line. Okay. So this is done. So now I will sudo make install -j6. So it will install my FFTW. Is it done. So now installation is done. Yes. Now I will go to gromacs.

So first I will uninstall the one and then I will do it again. So I have just removed the folder which is created. Okay. Using the command rm-rf. Okay. Then gromacs 4.6.5. That is all gone now. Yes. Okay. So now there is just the tar file left. So first we will untar it using tar. Okay. Space -xvzf gromacs. Okay.

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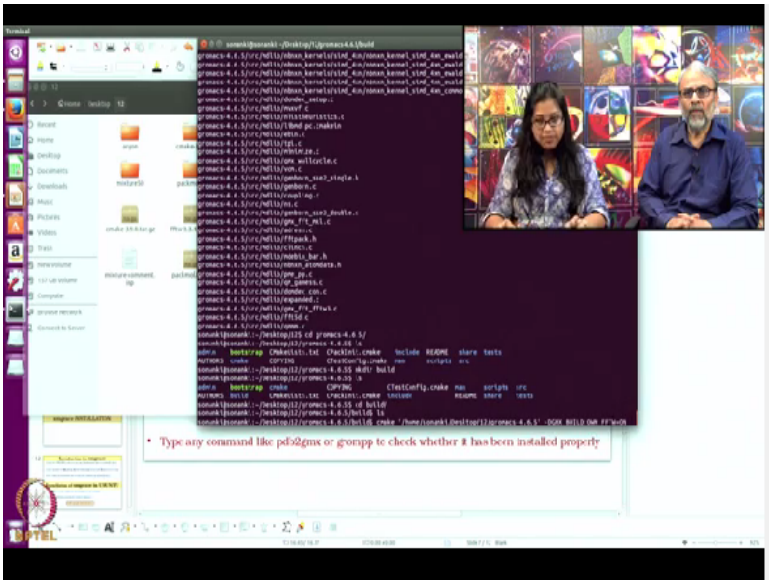

So untarring is done. Untarring your gromacs, okay. Yes, it is done. Yes. So now you go to the folder. Yes. Right and I have to create a directory build. So mkdir build. And going to build. Yes. And I will now go to build using the command cd. Yes. So cd build. Okay. And here I have to type this cmake and then I have to give the path of my. The new path. New path where gromacs is installed. So this is the one.

So I will just drag it here. Right. So it will give me the whole path. Okay. And then I will type space dgmx_own sorry _build. Okay. _own_fftw=on. Okay.

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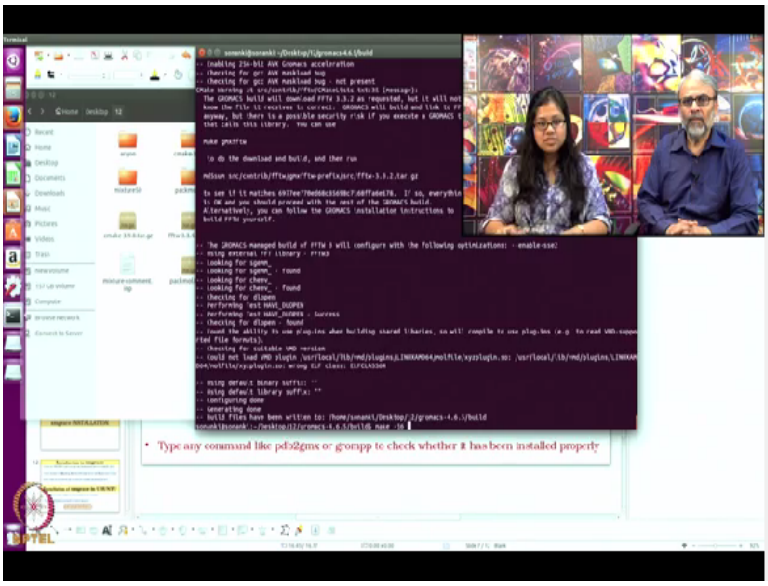

It had executed this step also correctly last time? Yes. So now I will make. Okay. So it is written there configuring done, generating done, right. Okay. So now I will make it make -j6.

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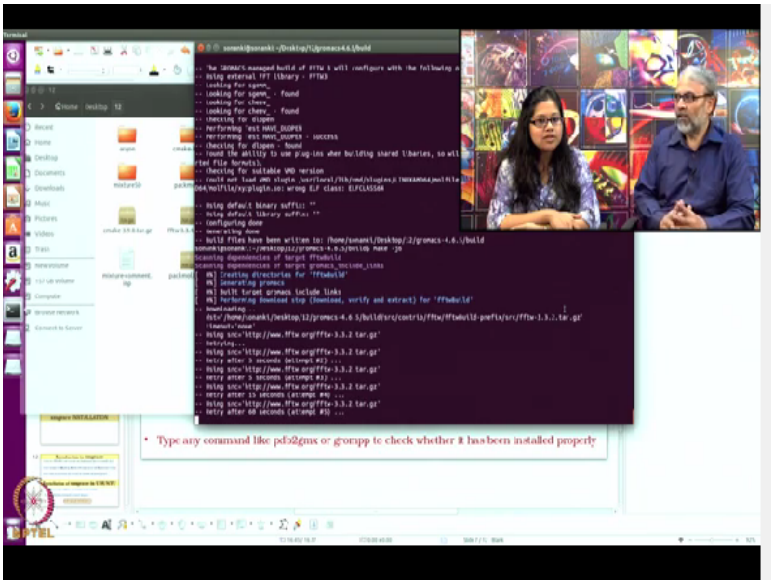

Okay. It is again showing the same thing, retry after 5 seconds. What are some of the other kind of problems you will come across. Generally, FFTW gives an error. Okay. Because of the some mismatch. May be because it has to be installed and the version has to be correct. Okay. So is it because the internet speed, is a problem now or you cannot say? I cannot say. Okay. No it is alright, it is good to get some trouble here because the user may get some trouble.

Yes, may be. While they are installing. Definitely. And anyway they can contact us if they have a

trouble. Yes. Okay. And are there some sites where you can? Yes, there is a. Post a problem. Gromacs site is there. Okay. Where it is a free site and you can post your problem and there might be some problems similar to that already posted earlier. So you can go there and there are answer given by some experts. Okay.

So which are the other problems you have faced, once you faced a problem with that wrong version of FFTW.

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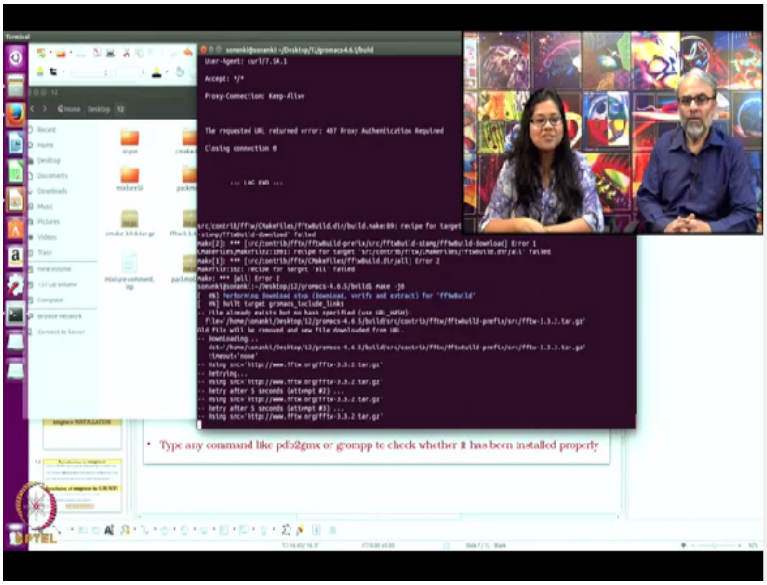

Yes, generally the FFTW gives the error. Okay. So why is the error here now? Same error, the, recipe for target src contribute FFTW, this failed, this downloading being failed. Okay. So then probably what we will do, we will recheck once again, whatever they have done. Yes. And start in the next session. We will, is it doing something better? No, it is just trying there. Trying the same thing. Okay.

So what we saw here so far, most of the steps that we executed went on very well. There is a problem in the last step of installing with the gromacs software. Yes. So this FFTW gives a trouble many times because the versions that are needed in this gromacs may not match what you have downloaded. Yes.

So what we will do today, we will go back and check what went wrong and in the next lecture,

we will start at this point and execute the installation. Then also show the advance simulation, water simulation as well as the mixture simulation. So we will conclude today's session and start next time at the point where we got stuck here. Thank you.