Foundation of Computational Material Modelling
Narsimhan Swaminathan
Department of Mechanical Engineering
Indian Institute of Technology Madras
Input Script for LAMMPS 3

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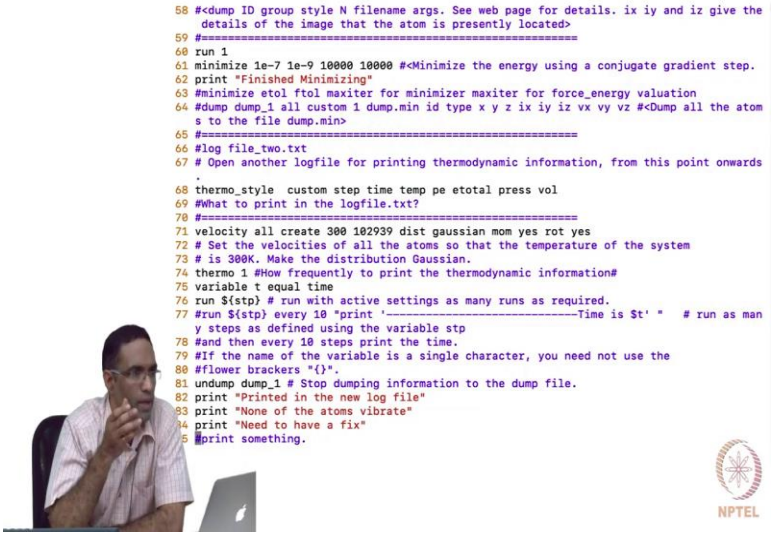

So good afternoon, take a look at the input file that we generated yesterday and so the first script that we just generated yesterday was a very simple script just to highlight the various commands. And like I mentioned this if you look at the dump file and load it onto Ovito, you might not see the atoms moving and reflect the fact that or reflect any temperature for that particular system. So what is basically happening is that it is not enough if you just give me initial conditions or the initial positions you are supposed to integrate the equations of motion so that the, the coordinates

of each and every particle and the velocities of each and every particle are actually updated with time.

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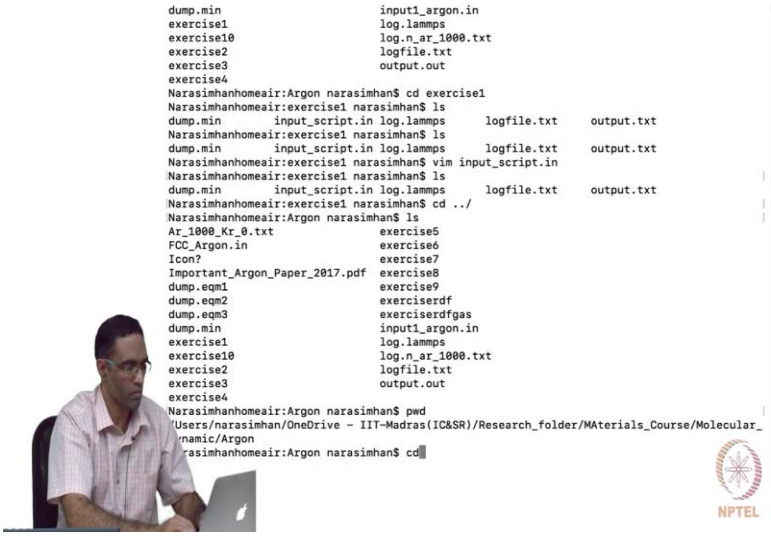

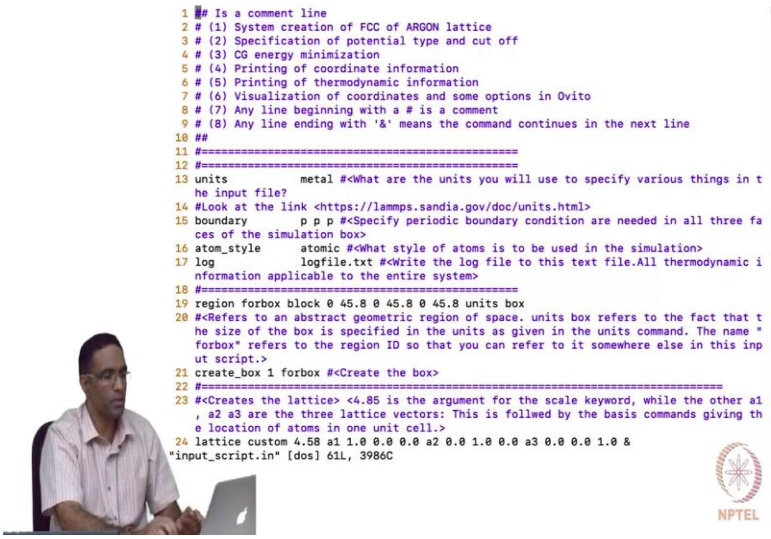

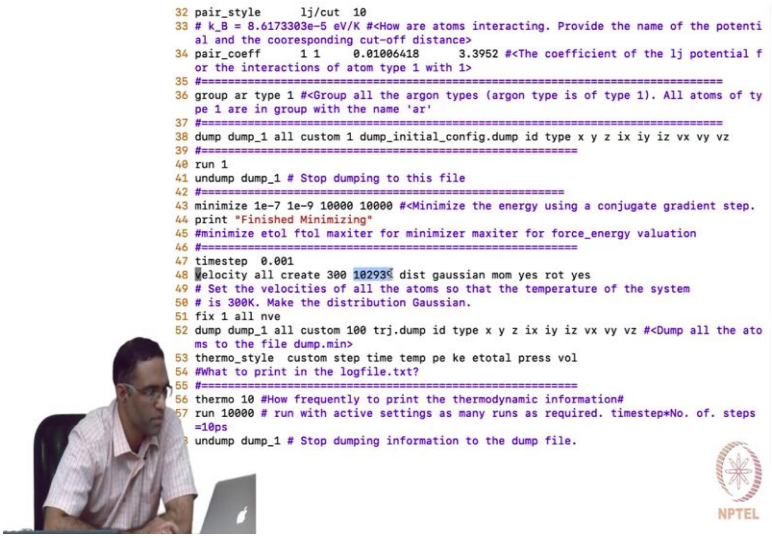

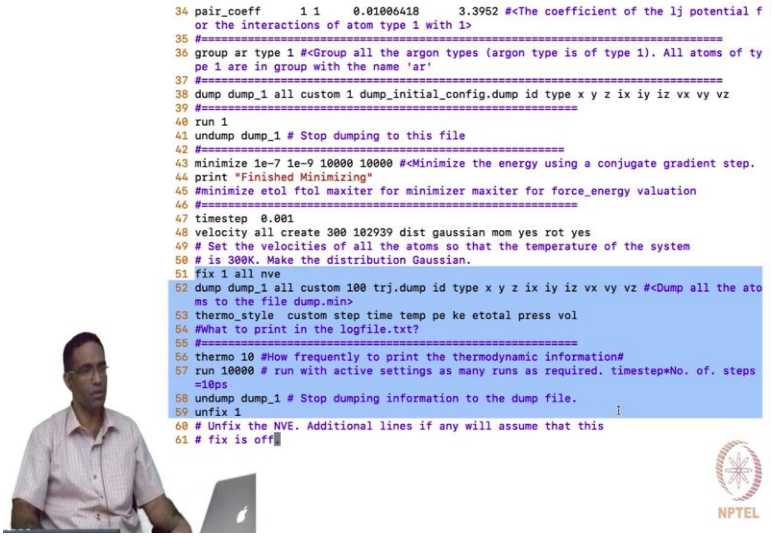

So we will now generate a slightly different version of the input file which is very similar to the previous one except that, now what I am going to do is after initializing the temperature to a set value, say 300 Kelvin and I am going to start integrating the equations of motion. For integrating the equations of motion you use what are offered to as fixes in LAMMPS. There are different kinds of fixes, each of which is meant for a different purpose. The simplest one is obviously an NVE integrator. So you are having a system, you are having a set of initial positions and initial velocities and now you are going to do that means, that means, what does it mean? It means that the initial energy, total energy of the system has been set.

And with that position you are going to start evolving the positions and the velocities of all the atoms in the system. So this is the input file. It is pretty much the same until here where I say velocity all create 300 Kelvin. This is a random seed. I want the Gaussian distribution and I want

to cancel out any rigid body translation and rigid body rotation. Then I say fix one all nve, which means this is actually the idea of the fixed which we want to refer to later on in the script. This is the set of atoms or the group to which we want to apply the fix or perform the integration.

So as you can see, you can actually not necessarily have all the atoms in a particular fix that you are using. So for example you could have a system and only the surrounding there you could you could choose, you could choose a surrounding shell of atoms in the simulation box and apply a different fix to the and apply a different fix to the set of atoms that present within that shell all that all that is possible. But in this case we are actually applying the fix to the entire set of atoms, all the atoms here and during the process of integration I want to dump once again the positions and the velocities of all the atoms in the system. And I want to do it every 100 steps and I want to do it in a file called a trj dot dump.

One of the things you should notice is that when you use a specific ID, for example earlier on the same file. I had used a dump command which looks like this. This is just to print the initial configuration of the system. I had used exactly the same dump ID. Now if I want to use the same dump ID, I need to undump it, stop it, stop the program from writing out information into that file, and then it allows me to use the same, dump ID. If I did not do this, if I said dump here and again used dump dump underscore 1, then it will throw up an error saying that this thing has already been used and it is going to happen only when it reaches this line.

So you need to make sure that you are not using the same dumb IDs or any IDs. For example, even the fix ID, you should not use one until and unless you have actually unfixed it stopped performing that integration process. So this fix command basically performs a nve integration, updates equations of motion, updates the positions and the velocities like I mentioned. And as it is doing, so it is going to print out the thermodynamic information every 10 steps and dumps the coordinates and the velocities every 100 steps. Now this is run for about 10000 steps, so 10000 steps means 10000 multiplied by 0.001 which, results in about 10 picoseconds of simulation. And that is level of 4000 atoms. So this takes a little bit of time to run. So I am really, so if you want to see how it runs, we can.

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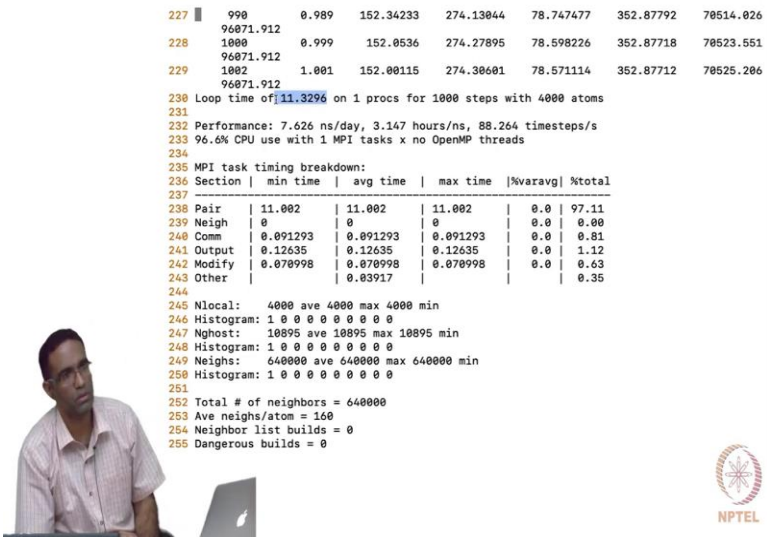

So let me run it for just one picosecond. It is done. So when you look at log file, some additional information is also available. Kind of tell, it kind of tells you how long the simulation has actually taken to run. And this is useful for you to decide loop time of 11.3296 on one processor for 1000 steps with 4000 atoms. So this is a total number of seconds. It does take into one on this computer. And this is going to be a very important information for you to decide, you know, how long or estimate how long your simulation is going to run.

You should also remember that a molecular dynamic simulation does not take time only to simply run but every time you are asking you to output data also it is going to consume some time. So if you are going to ask you to dump a million the positions and the velocities of a million atoms every step then that input output operation is going to consume back. So that is also an important thing for you to keep in mind while you are setting up your simulations.

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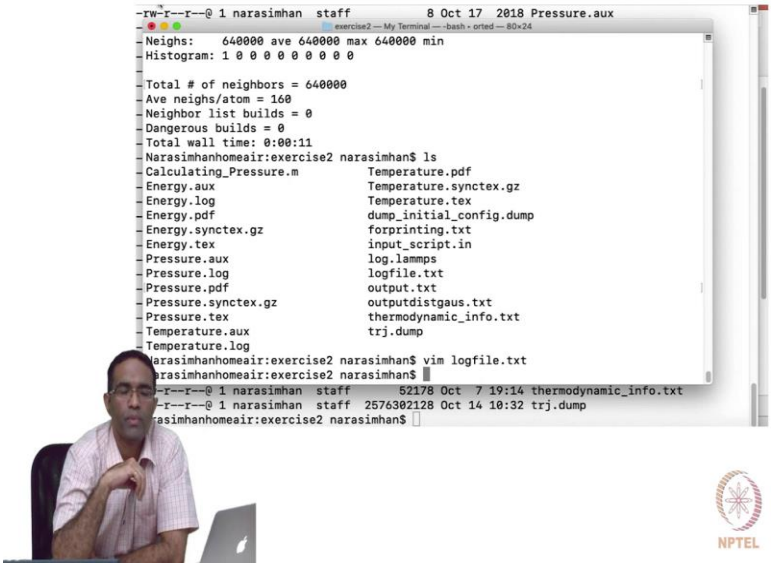

So what do we do now? We set the temperature to about 300 Kelvin. That means we have initialized the velocities of all the systems. We have all the atoms sitting in their equilibrium positions. And then we have set the, the velocities of all the atoms to reflect the 300 Kelvin and then we have started integrating the equations of motion. So the question now is what does the temperature turn out to be? What does the pressure turn out to be? And what is the energy of the system? These are some of the things that we can look at. The first thing is let us look at the temperature. So I have already finished these calculations I have done it for a longer period of time just for illustration purposes. So I will not run it again here for that long time.

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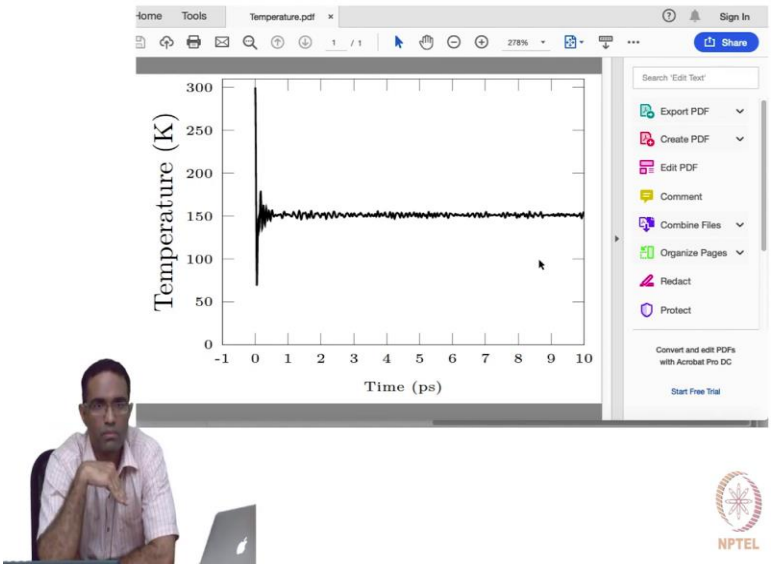

So this is the temperature profile. So what are you seeing here? You started, you initialize the temperature at 300 Kelvin. So the first step, the first point is at 300 Kelvin. But as a temperature as the simulation began to evolve you basically started, you started reaching some other temperature and it happens to be half of what you started off with, close to half of what you started off with. You can experiment this with many different temperatures. For example, if you set the initial temperature to be 500 Kelvin it will, it will and if you did exactly this it will converge to 250 Kelvin.

If you started off with a 450 Kelvin it will converge to 225 Kelvin. So the set temperature is actually not the temperature that it reaches to under equilibrium conditions. The reasons there are, there are very rigorous derivation which can be shown as to why this is taking place. So especially for systems where the interaction between the atoms is governed by a harmonic potential. Harmonic potential means just a linear spring. You can actually show that using a rigorous derivation that the set temperature is actually twice the temperature that it reaches at equilibrium.

Even for systems which do not have this where the interaction potential is not harmonic, if the atoms are going to be vibrating about their mean positions very little, even though the intra-atomic potential may be something as complicated as the Lennard-Jones within the vicinity of equilibrium, it is almost harmonic. So even then you will be able to see this set temperature being twice that of the temperature but it reaches equilibrium. So what do you think is the main reason for this? Why does this happen? Why should it be half? What happens?

Student: Energy conservation between kinetic and potential energy

Professor: Correct. Yeah. So initially, you initialized only the kinetic energy part of the system. You did not do anything to that potential energy part of the system. So when all the energy that was given to it was kinetic energy. As the system evolves the energy is being distributed between the kinetic energy part and the potential energy part. Consequently, the temperature at which the temperature the equilibrium temperature to which it reaches is less than the temperature at which you set.

And because this is almost harmonic it happens to be T set, the equilibrium temperature happens to be T set divided by 2. So if you want a system to be equilibrated at 300 Kelvin just be initializing the velocity to 300 Kelvin it is actually not sufficient. And for more complicated

systems your temperature may not necessarily oscillate about T by 2. So you will have to do something in order to set the temperature of the system and bring it up to the required temperature that you need. That is basically a that is where we talk about velocity rescaling or using thermostats in order to rescale the temperature of the system.

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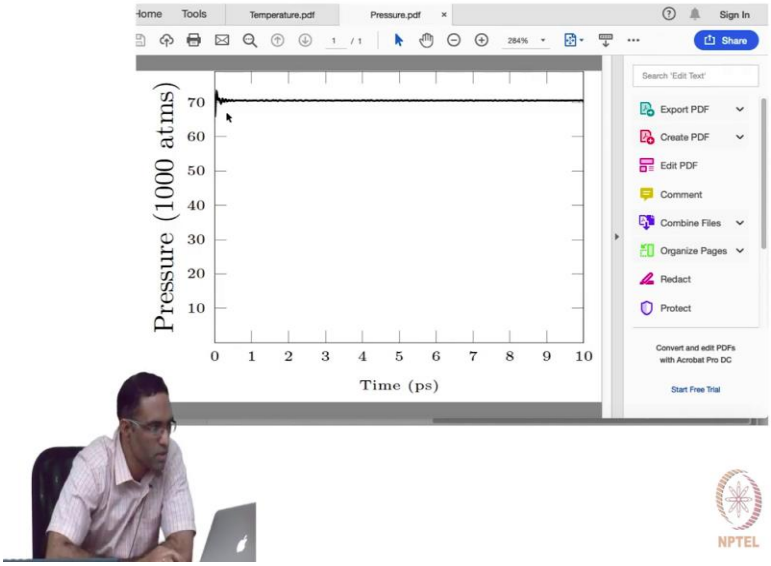

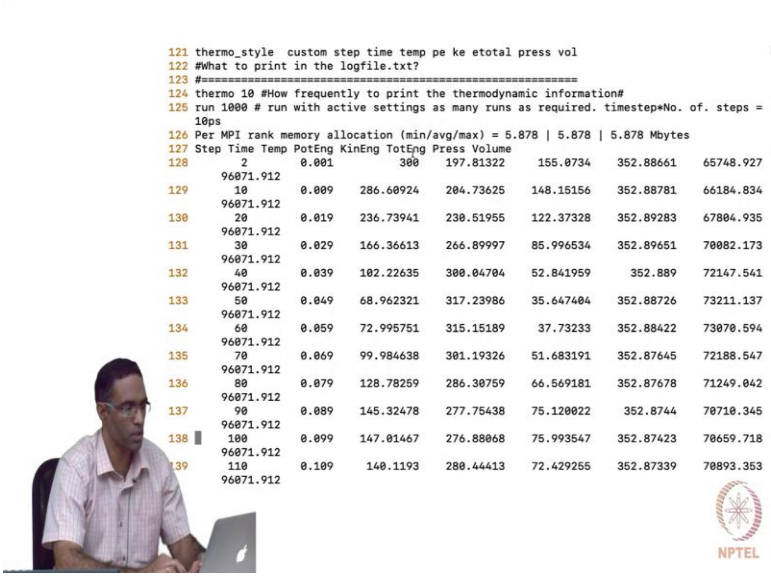

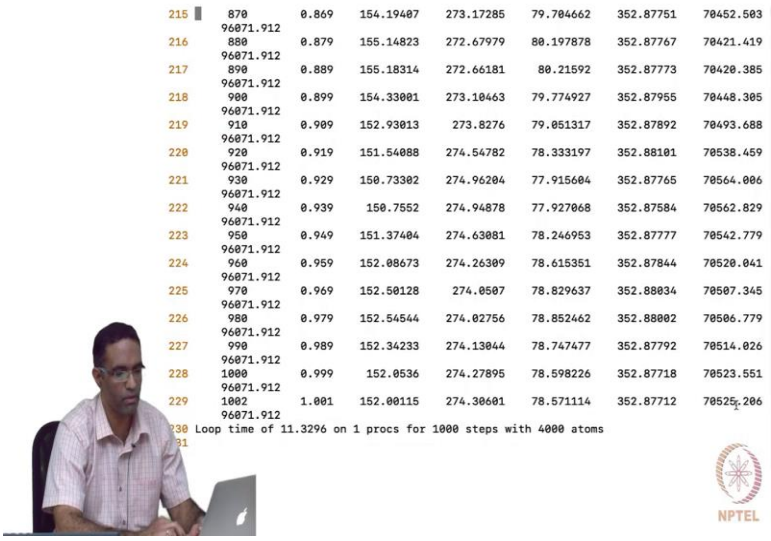

So the pressure of the system is about 70000 so you should take a look at the log file. So this is step time, temperature, potential energy, kinetic energy, total energy, pressure, volume. So pressure is this. So which is this and it converges to some 70525 which is in terms of bars. So I just divided it by 1000 and plotted it in terms of 1000s of atmospheres and that is what you are seeing there that is the pressure and the volume is obviously fixed and it will be exactly what you started off with because you are not allowing the volume of the system to change. This is in fact NVE integration.

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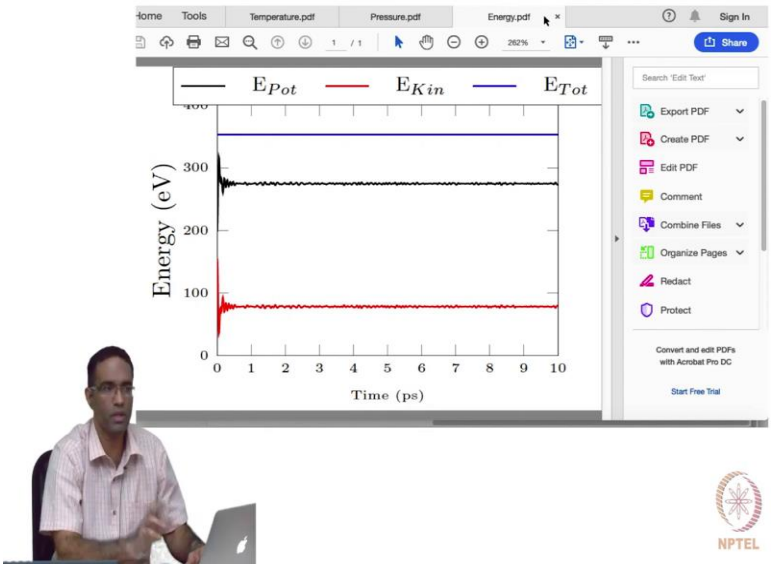

If you look at the energy, so this is the energy distribution. So you started off with this is the potential energy part, this is the kinetic energy part. This is what you gave initially and then it

has redistributed itself between the various degrees of freedom that is available to the system. However, the total energy of the system is perfectly a constant because you are obviously just the, the initial, kinetic energy that you gave by setting the velocities to 300 Kelvin is actually the total, governs the total energy of the system, so that is what it is going to be.

After that the energies are being distributed between the potential and the kinetic energies and you have something that looks like this. So there is a little bit more statistical mechanics that one can do in order to understand why the energies are being distributed in a particular manner. And also for the and also the reason as to why the final equilibrium temperature turned turns out to be T set divided by 2. So, if possible I will just post the derivation in the notes that I am sharing with you. That should be clear from that. So are there any questions in this?

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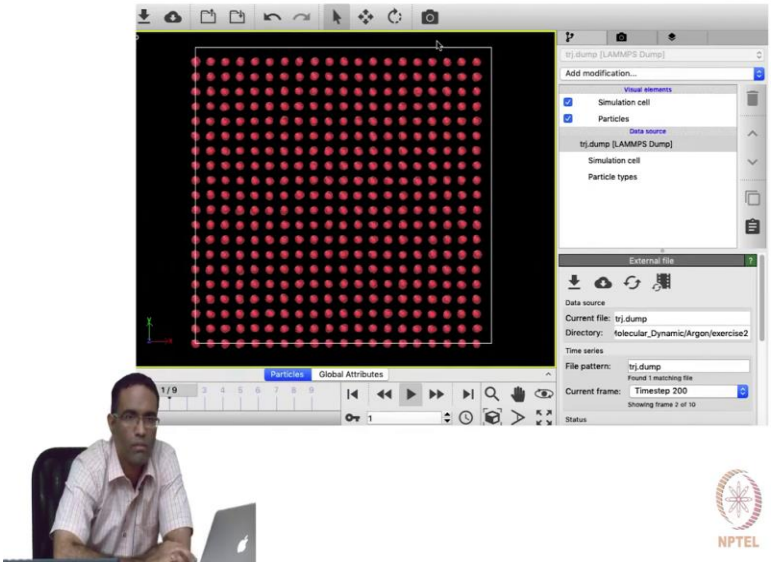

So now let us take a look at our trajectory and see if, so you can see some moment in contrast to what you saw yesterday where the atoms they were not moving at all. So this is essentially because now the atoms are being integrated and you are getting new positions and velocities for all these atoms and they are juggling about their min positions. So this is how you can start to visualize your MD simulations using Ovito, you just have to drag that particular file dump file into this window and it will open up. Are there any specific questions regarding this?

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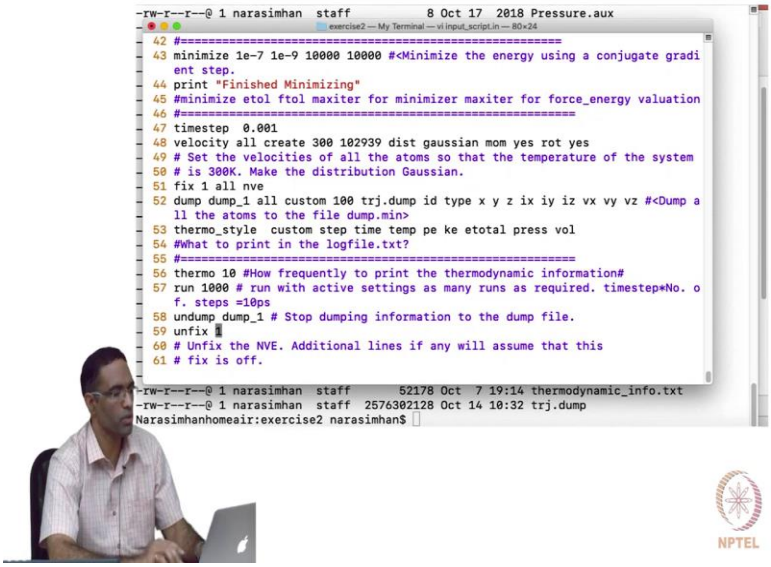
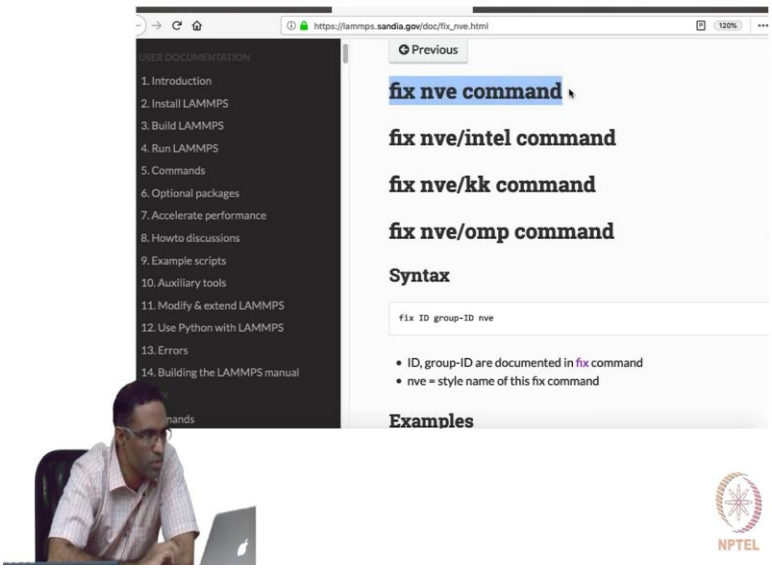
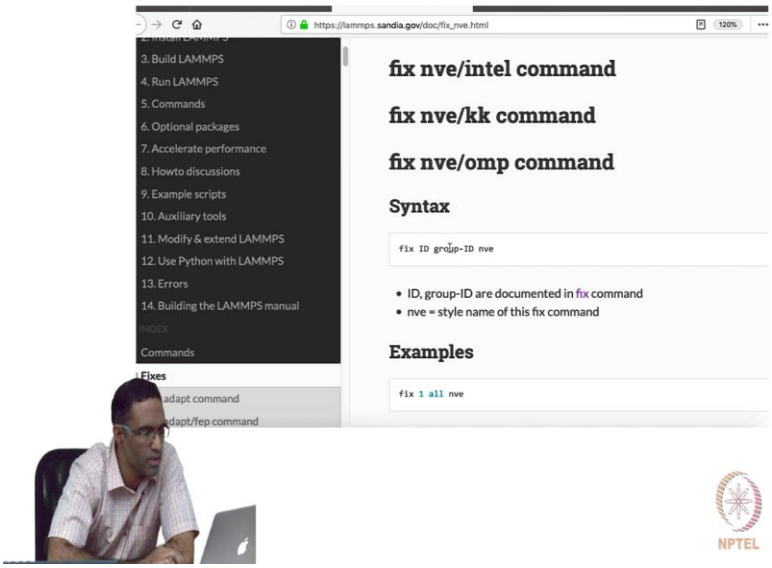
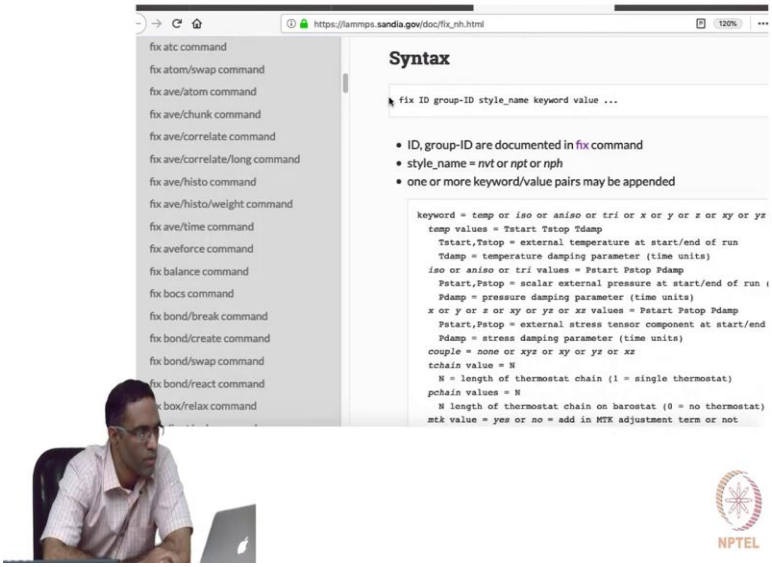
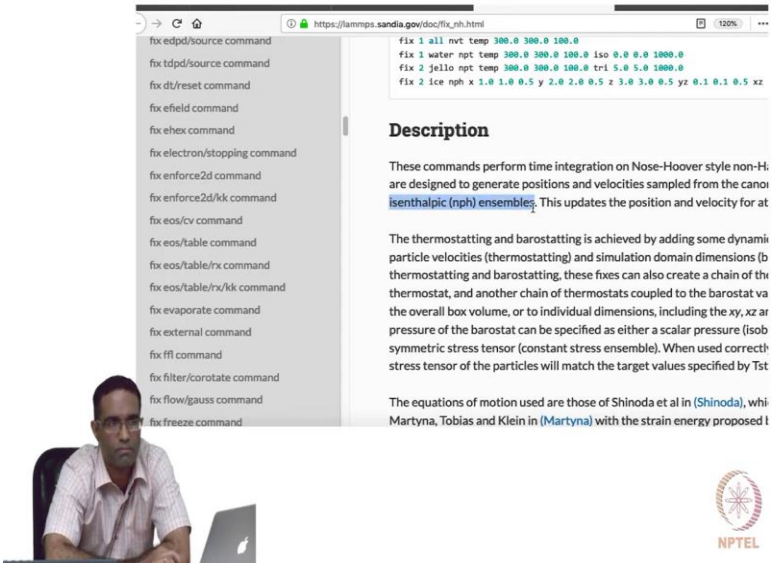





https://lammps.sandia.gov/doc/fix_nve.html
3. Build LAMMPS
4. Run LAMMPS
5. Commands
6. Optional packages
7. Accelerate performance
8. Howto discussions
9. Example scripts
10. Auxiliary tools
11. Modify & extend LAMMPS
12. Use Python with LAMMPS
13. Errors
14. Building the LAMMPS manual
Commands
Fixes
fix nve/intel command
fix nve/kk command
fix nve/omp command
Syntax
fix ID group-ID nve
ID, group-ID are documented in fix command
nve = style name of this fix command
Examples
fix 1 all nve


https://lammps.sandia.gov/doc/fix_nh.html
fix atc command
fix atom/swap command
fix ave/atom command
fix ave/chunk command
fix ave/correlate command
fix ave/correlate/long command
fix ave/histo command
fix ave/histo/weight command
fix ave/time command
fix aveforce command
fix balance command
fix bocs command
fix bond/break command
fix bond/create command
fix bond/swap command
fix bond/react command
Syntax
fix ID group-ID style_name keyword value ...
ID, group-ID are documented in fix command
style_name = nvt or npt or nph
one or more keyword/value pairs may be appended
keyword = temp or iso or aniso or tri or x or y or z or xy or yz
temp values = Tstart Tstop Tdamp
Tstart,Tstop = external temperature at start/end of run
Tdamp = temperature damping parameter (time units)
iso or aniso or tri values = Pstart Pstop Pdamp
Pstart,Pstop = scalar external pressure at start/end of run
Pdamp = pressure damping parameter (time units)
x or y or z or xy or yz or xz values = Pstart Pstop Pdamp
Pstart,Pstop = external stress tensor component at start/end
Pdamp = stress damping parameter (time units)
couple = none or xyz or xy or yz or xz
tchain value = N
N = length of thermostat chain (1 = single thermostat)
pchain values = N
N length of thermostat chain on barostat (0 = no thermostat)
mtk value = yes or no = add in MTK adjustment term or not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fix edpd/source command
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fix dt/reset command
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fix electron/stopping command
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fix eos/cv command
fix eos/table command
fix eos/table/rx command
fix eos/table/rx/kk command
fix evaporate command
fix external command
fix ffl command
fix filter/corotate command
fix flow/gauss command
fix freeze command
fix 1 all nvt temp 300.0 300.0 100.0
fix 1 water npt temp 300.0 300.0 100.0 iso 0.0 0.0 1000.0
fix 2 jello npt temp 300.0 300.0 100.0 tri 5.0 5.0 1000.0
fix 2 ice nph x 1.0 1.0 0.5 y 2.0 2.0 0.5 z 3.0 3.0 0.5 yz 0.1 0.1 0.5 xz
Description
These commands perform time integration on Nose-Hoover style non-H
are designed to generate positions and velocities sampled from the canoi
isenthalpic (nph) ensembles. This updates the position and velocity for at
The thermostatting and barostatting is achieved by adding some dynami
particle velocities (thermostatting) and simulation domain dimensions (b
thermostatting and barostatting, these fixes can also create a chain of th
thermostat, and another chain of thermostats coupled to the barostat va
the overall box volume, or to individual dimensions, including the xy, xz ar
pressure of the barostat can be specified as either a scalar pressure (isob
symmetric stress tensor (constant stress ensemble). When used correctl
stress tensor of the particles will match the target values specified by Tst
The equations of motion used are those of Shinoda et al in (Shinoda), whi
Martyna, Tobias and Klein in (Martyna) with the strain energy proposed l

So after I ran it for about a 1000 steps, I am stopping the process of writing out information into the dump file and I am also performing an unfix. That means I am going to stop initializing that command, unfix one. You can have any, any arbitrary names for the fix ID and I am unfixing it once I am done with the simulation. So let us take a look at the LAMMPS documentation to see other types of fixes which may be present. So what we saw here was fixed nve command. It is a basic integrator. And you can have different types, but this is what we most commonly use. So it is just fixed.

There is the ID for the fix, the corresponding group ID and followed by nve is what you need in order to run this. But this is just going to perform a simple integration, there is nothing more to it. But if you want to now bring the system to a specific temperature, then you need to couple the existing temperature for some sort of an external bath. And that bath will actually is supposed to constantly pump in heat to the system so as to raise its temperature to the required value. This process is referred to as a thermostat. So you have a thermostat, Nose-Hoover thermostat as we call it.

And that is done by using what is referred to as the nvt command, fix nvt command. Again, same. So fix ID, the group ID, there is set of all atoms for which you want to apply this fix, the style name. So which can be nvt or npt or nph. So in nvt, the only thing that you want to control is a temperature whereas in npt you can control or specify the particular value of pressure and temperature that you want the system to reach. And in nph, it is a combination of pressure and enthalpy, isenthalpic ensembles can also be realized. So depending upon what you are using, you know, whether you are using nvt or npt or nph, the keyword and the corresponding values that you have to do can actually be quite different.

Student: Sir h stands for?

Professor: Enthalpy, isenthalpic.

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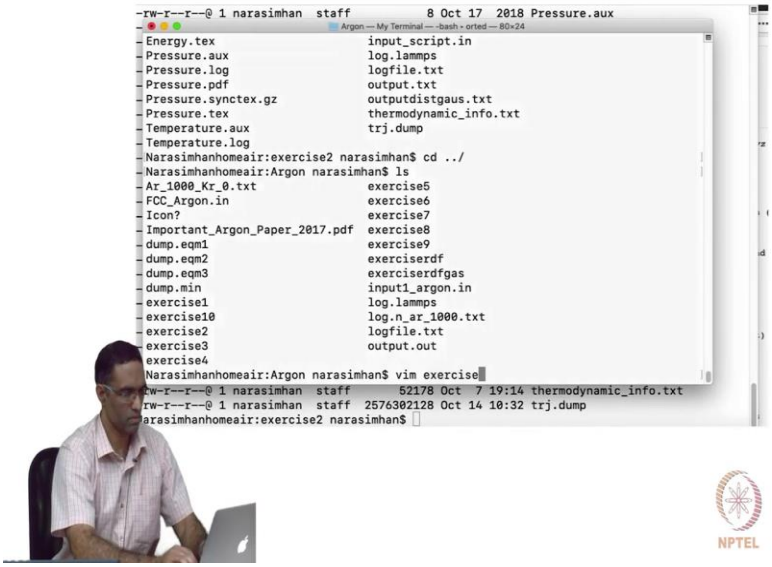

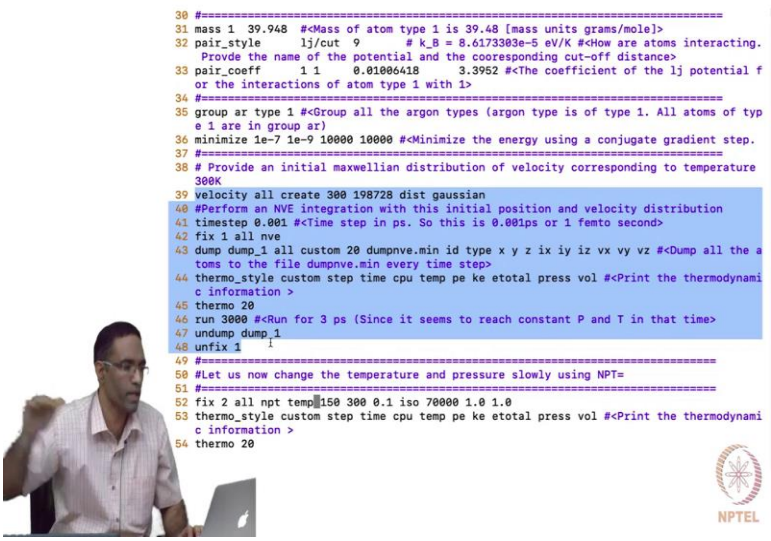

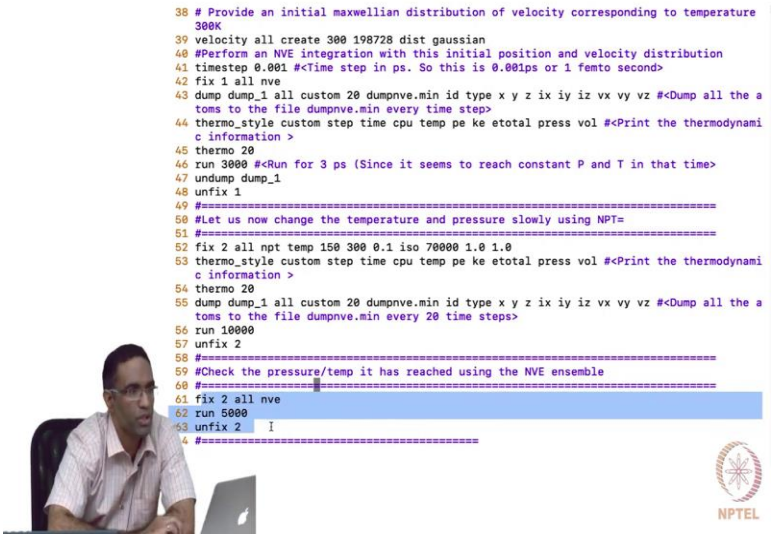

So if you have, so let me open that, let me see if I have a. So in this case, what I do, almost everything is the same. I provide initial velocity. And I print out some information here. Now I want to change the temperature slowly and the pressure slowly. So fix 2 all. I use npt, I changed the temperature of from, you remember when we just created all the a, when we just created the velocities corresponding to 300 Kelvin and ran the nve simulation. So this is actually going to result in ending the temperature at around 150 Kelvin.

So now I want to perform an exercise where I slowly ramp up the temperature from 150 Kelvin to actually 300 Kelvin. So fix 2 all npt. And I say that my start temperature is 150 Kelvin and I want to end at 300 Kelvin. And they specify a parameter called tdamp. And then I specify iso, which means I want to iso iso isometric, metrically apply the pressure, which means the pressure is going to be the same in all the directions.

And the starting value was 70000 and I want to bring it down to 1 bar. It was 70000 bar previously, but now I want to bring it down to 1 bar. So I want to bring it down to say atmospheric conditions, 300 Kelvin and one bar atmospheric pressure. And I had to specify something called is it pdamp, we will come to what this P damp in a little bit but let us first see what are the results of this simulation. And then I run this again to about 10000 steps, I unfix it and then perform once again an nve simulation.

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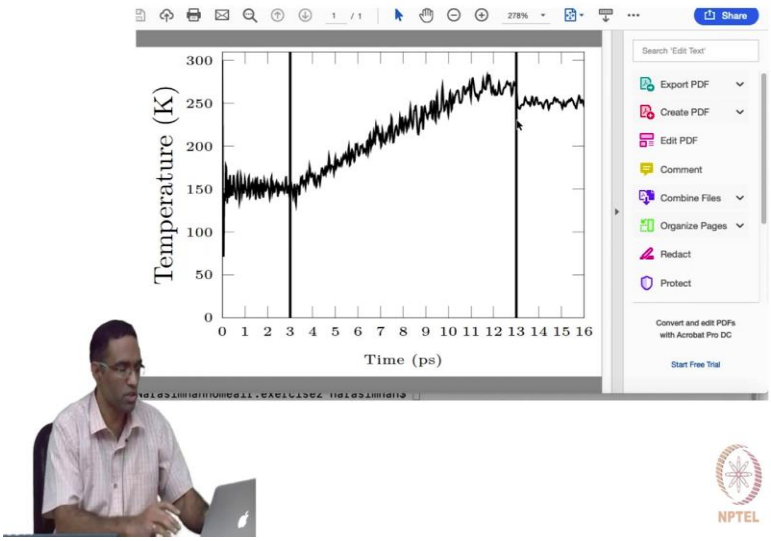

So if I ran that simulation, so this is what is going to happen. So the first set that you are seeing here is for the nve part where the temperature was just set to 300 Kelvin and then it came down to 150 Kelvin. And then this is the part of the npt where I am slowly ramping the temperature from 150 Kelvin to 300 Kelvin over 10 picoseconds. However, after that I ran a nve. Why I do it, why did I run the nve? npt is what npt or nvt, either of them are essentially involving the system, exchanging heat or some sort of work with the environment so as to bring it up, bring up the pressure and the temperature to the required value.

Now I am doing this for some time. I am continuously pumping in heat or removing heat or doing some mechanical work on the system by resizing the boxes so as to reach the required temperature or the pressure. I am doing it for some finite time. So in this case it is 10 picoseconds but after that, I do not know if at the end of 10th picoseconds the system has actually reached equilibrium. So what is the definition of equilibrium, what is the definition of equilibrium? When, when a something reached the thermodynamic equilibrium? How will I find out?

Student: Sir means when the thermodynamic parameters of temperature, pressure and chemical potential do not change with time of the system, then it have reached thermodynamic equilibrium.

Professor: So now if I have a, if I have a rod, the temperature on the left hand is say 300 Kelvin, then the temperature on the hand is 500 Kelvin, after it has reached to steady state, the temperature at any single point never varies with the time.

Student: But still it is not in equilibrium state.

Professor: But still it is not an equilibrium state.

Student: No, it is not an equilibrium state because temperature is not same throughout the system.

Professor: The temperature is not same throughout the system. Another way of looking at it is if I but how will you actually find out of the system as in equilibrium? The only way to find out is to isolate the system from the surroundings. You take the system and isolate it from the surroundings. If after isolating from it surroundings nothing inside changes then the system is said to have reached equilibrium, is said to have been in equilibrium with its surroundings. Is not it? If you have a body and it is at constant, at constant temperature, then if you isolate it from the surroundings and then look at the temperature it would be the same if it has actually, if it was actually in equilibrium with the surroundings.

This bar which was having you know, different temperature on either sides. If I take it and I isolated it from the surroundings immediately the temperature will start changing inside because there will be heat flow in order to make the temperature uniform through the system. So the manner in which equilibrium is checked is by isolating the system from the surroundings. So that is exactly what I am doing here. So after having this npt fix for some time and allowing the system to exchange heat or mechanical work with the surroundings, I am stopping that fix and starting nve.

And this nve is actually, an isolated system and I am checking if the temperature and the pressure are what I want. Now it is what happens when I stopped it and ran the nve simulation, the temperature was a little bit lower. It was somewhere around 250 and it has not yet reached that 300 Kelvin value that I wanted. It has not reached 300 Kelvin that I wanted, but it has reach some other value. Why is…

Student: Because we programmed it to run till 300.

Professor: Yeah, but, but, but what is happening is so it is constantly pumping in some energy but the time for which I have done it is not sufficient enough for it to actually reach that temperature.

Student: Sir, so if we increase the number of iterations in the simulation the command we say the pressure is 1 bar and the temperature is more than 300, make the iterations, more iterations.

Professor: No, that is not what I have done.

Student: Yeah you did like less iterations. So if I say like I run it for 20000 iterations and if I mentioned the same command, will it breakout when the…

Professor: It will not breakout. It will run, it will keep running it, it will not break out unless you explicitly tell it to break out. It is going to run for as many times step that you have specified here.

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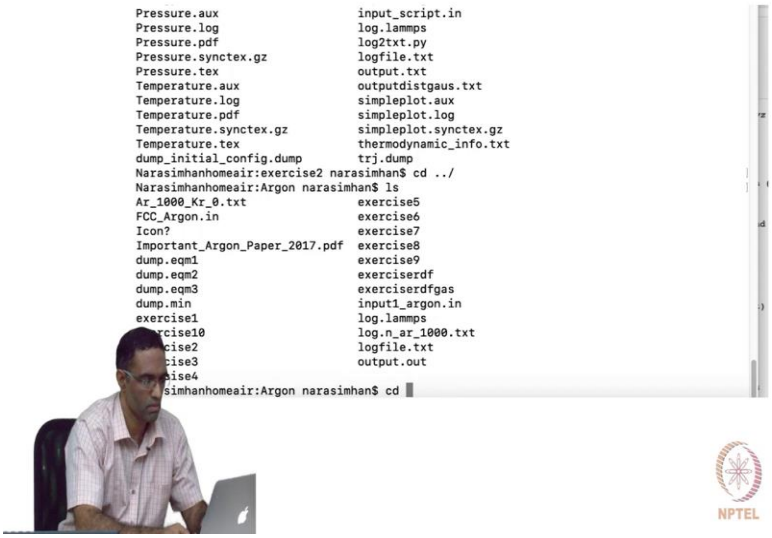

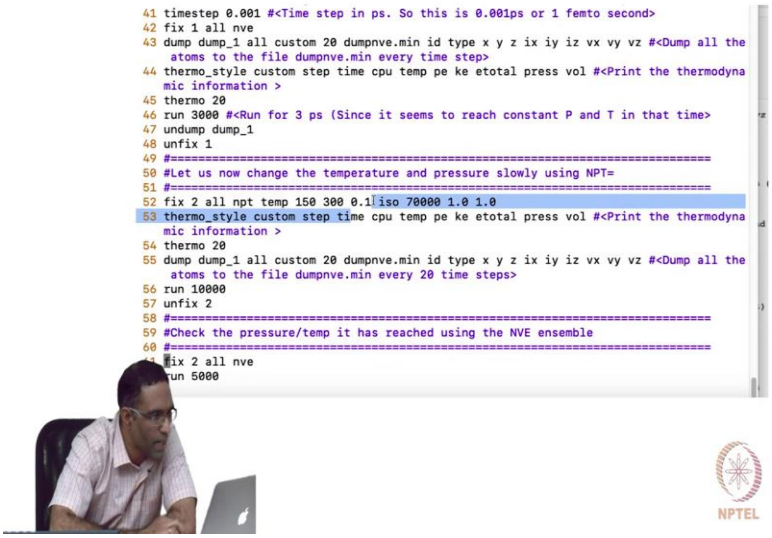

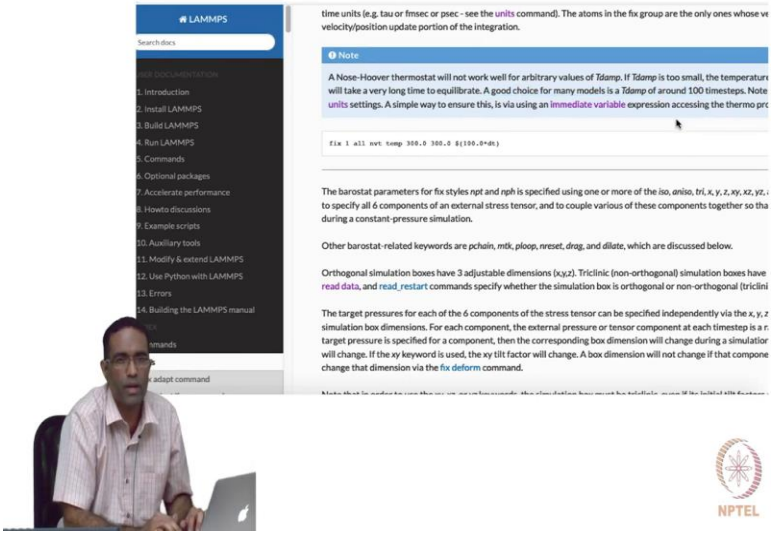

So let us take a look at the input script once again. So yes or it should continue to pump it so as to maintain that temperature.

Student: Can we input a heating rate?

Professor: No, no you cannot. It is, when you specify the temperatures it is going to do it. The rate you can that is what the T damp and the P damp do. So I do not have whether I have examples for that in today's class. But let me take a look. So let us take a look at the input file before we answered that question. So in the, the npt command basically took a couple of different it took this T damp, which kinds of tells it how fast you want the temperature to actually reach the value that you require and P damp is actually how fast you want the pressure to actually reach the value that you require.

Too high value essentially means that you are forcing the pressure to come to the value that you require very quickly and you will see huge fluctuations in the pressure. And if you give too lower value then it will take a very very long time for it to actually reach the pressure that you are requesting. So usually there is a Thumb rule that one uses when you are using these nvt and npt commands. So here, A Nose-Hoover thermostat will not work for arbitrary values of T damp . So usually a good choice for T damp is around a 100 time steps. So our time step was 0.001. So that is the reason why I have given 0.1 there.

And for similarly for P damp it is about a 1000 times that time step which is about 1. So that is why you see a value of p damp to be equal to 1 which is the standard way of which is the lammps suggested way of giving the values for T damp and P damp. Again, what exactly T damp and P damp are doing to the equations of motion is not something that we are going to be teaching here. So that involves actually coupling the system to an external bar and solving the equations of motion along with some additional degree of freedom. This T damp and P damp are going to control how quickly the requested temperature and the required, and the required temperature are going to match.

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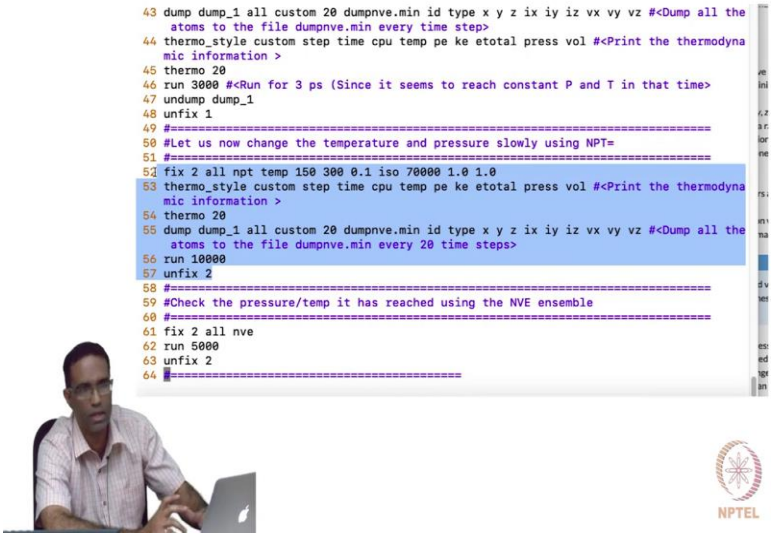

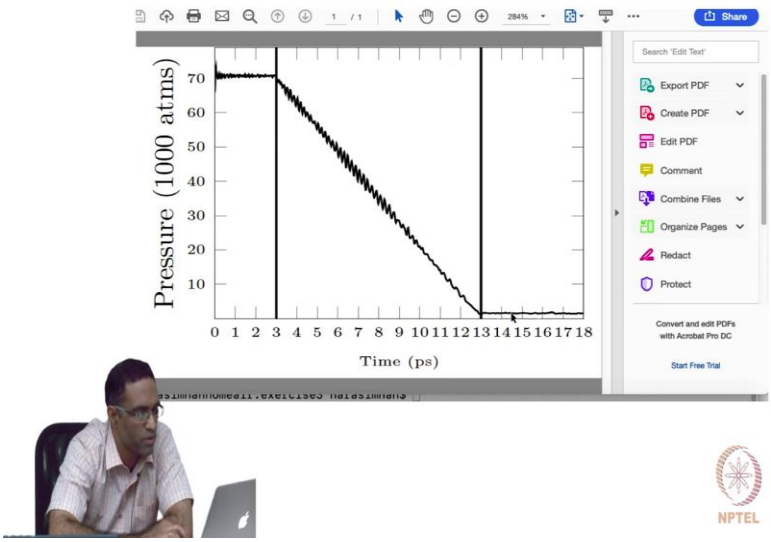

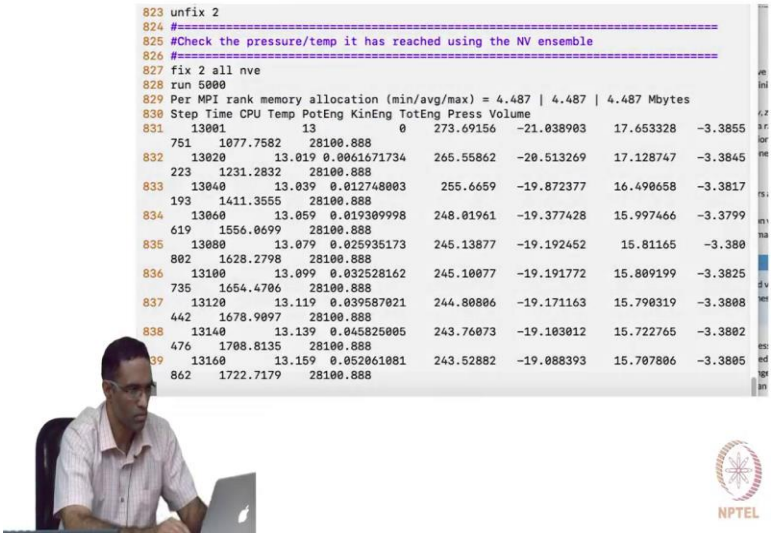

So I have after running this npt, I actually stopped it and only then ran the nve. So a good way to actually check if your system has reached equilibrium is actually to after performing the npt or nvt whatever you want, stop that, stop that a fix by doing this unfix command and check all the parameters if they have reached the value that you requested. So I do not know what the pressure value reaches. So pressure value is this. So you see those 70 and then it is come down and it is reached some specific value. I really do not know if it is 1, but it is possible that it is 1, it is not really 1 yet. So that is the way you check if your system has reached equilibrium.

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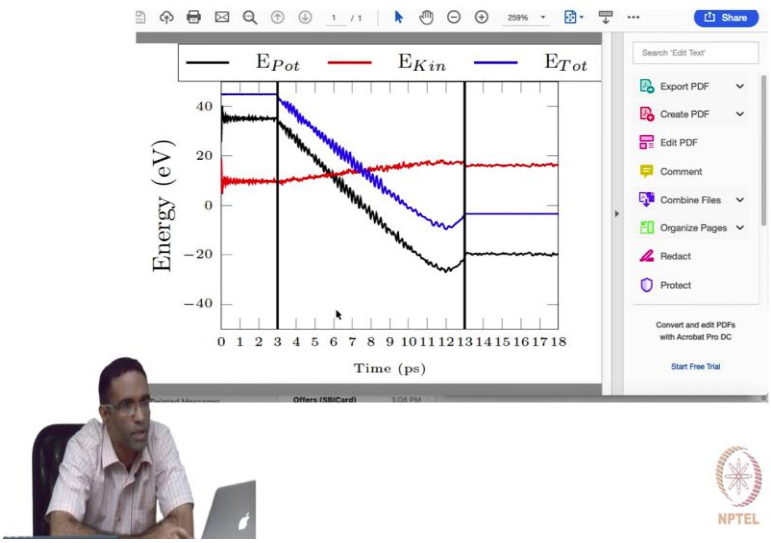

And this is the way the energy basically vary, so initially, your, this is the part where you do a pure nve initially. So this is the total energy. This is the potential, this is a kinetic energy. And then you are slowly increasing the temperature. So the kinetic energy increases and the potential energy is decreasing. You are decreasing the pressure of the system from huge value. And then after 10 picoseconds you have stopped doing anything and again running nve.

So you see the kinetic energy being constant, almost constant, the potential energy being almost constant, total energy being almost constant. So during this period because you ran npt you are expecting one thing, you are expecting the box, the simulation box to actually become huge because you have what you have done? You have decrease the pressure from 70000 bar to have a pressure of only about 1 bar.

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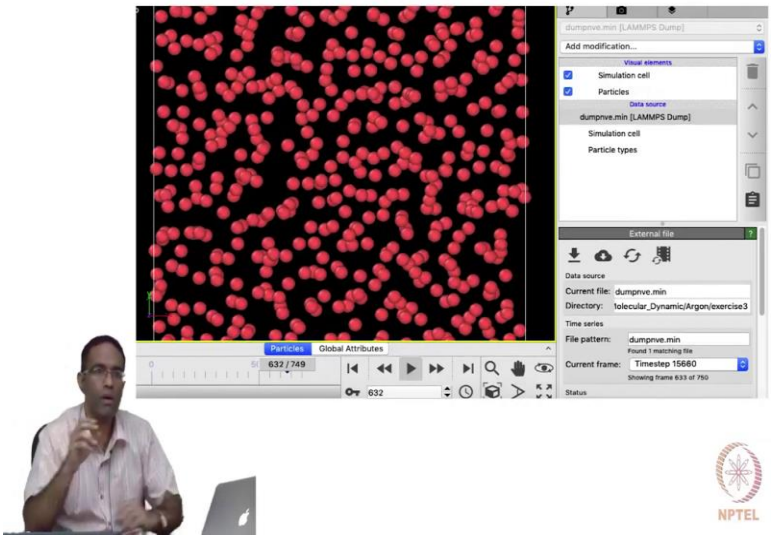

So let us take a look if, you saw that, did you see the box actually increase in size?

Student: Due to the decrease in pressure, right?

Professor: Yes. So the when you do nvt alone, the volumes is all fixed, the temperature only the heat input is given. When you do (nv) npt, you are controlling both the temperature as well as the pressure consequently to have the pressure that you want, the volume of the entire simulation cell will be adjusted.

Student: Here in nvt simulation N V and T are remaining constant?

Professor: Yes.

Student: N is the number of atoms?

Professor: Yeah.

Student: In npt simulation, N is constant, but pressure and temperature are changing?

Professor: They are not changing. That is a good point. So in npt, actually what you mentioned is, the statistical, statistical mechanically the pressure and the temperature of the ensemble is fixed. That is the macro state. But what you are trying to do in molecular dynamic simulation is you do not really know the positions and the velocities are or equilibrium configurations that the system must have at that pressure and temperature. You do not know how the velocity should evolve or how the position should evolve.

So what you are doing is you are starting off with some arbitrary state and using this npt fix to actually kind of training the system to reach that pressure and temperature. So here, the use of npt is not exactly fixing the pressure or fixing the temperature. It involves changing the pressure and changing the temperature to some fix level. Hopefully if you have done it long enough time, your pressure and temperatures will reach the value that you have requested.

Student: So the final value specified are the ones where you wanted to equilibrate?

Professor: Where you want to equilibrate to, to which you want the system equilibrate to.

Student: And in nvt simulation, N and V are fixed but I want to keep the equilibrium at the …

Professor: That value, that is right. So this is more like a…

Student: The ramp part is not important to us?

Professor: The ramp part is not important. You can start off and end with the same value. So these are given for different reasons. So if you want to do any specific temperature rate and all that, then you can do that. Usually we start off with the same temperature and in the same the temperature and it will equilibrate to that particular temperature if you have trained it up, if you have given enough time steps for it to… work?

Student: So for real objects like if I am having the piece of iron in this room that pressure on that pieces, one atmosphere because that is the pressure exerted by the atmosphere on that piece of iron. But in a molecular dynamic simulation, the same, the simulation was which we are defining it is being repeated in all three directions because of periodic boundary conditions.

Professor: Correct.

Student: And the pressure which is being calculated by the code, because of the running of code, that is the pressure experience by…

Professor: It is a pressure exerted by the molecules on a container on the size of the simulation box.

Student: The pressure exerted by the molecules?

Professor: On the side. That is the definition of pressure. What is pressure actually? If you, if you talk about, let us talk about the pressure of an ideal gas inside a container. What does mean by pressure?

Student: The pressure exerted by the…

Professor: By the molecules on the force with which the hit the surfaces of the molecules is what is constituting the pressure. So that is this, this is that pressure. Any other questions? So now you can go back. I will upload this and you can play with, play with it a little bit and try to see if you are able to show pv is equal to, yes?

Student: Sir when we are talking about the equilibrium, do you mean by every single particle in the box has the same energy, I mean…

Professor: No at equilibrium, no, it need not have the same energy.

Student: And what exactly do you mean by raw material do not change its space?

Professor: The particles have, the velocities of the particles have (been) are, for example, if you are talking about an ideal gas, then add equilibrium, the velocities of all the particles should be such that they have some the Boltzmann's distribution. So a equilibrium property is for the entire system the bunch of the entire atoms so it is not for each, not for each atom. In fact, we saw in statistical mechanics there it is in fact not the same for all particles.

Student: So when the system reaches thermodynamic equilibrium is that happens when thermal equilibrium, mechanical equilibrium, chemical equilibrium are actual reached?

Professor: yes.

Student: So chemical equilibrium is reached or chemical potential is same for all the system and does not change with time.

Professor: Yeah.

Student: So thermal equilibrium is reached when temperature remains same throughout the system and does not change with time and mechanical equilibrium means pressure remains same throughout the system and does not change with time. So if the temperature remaining same throughout the system, it simply means that the average kinetic energy is not changing as we go one point to another but the individual particles may have different kinetic energies.

Professor: That is what I am saying. Yes. It may not be the same. It is only the average. The equilibrium is defined only for the average, for the entire system. So now will you be able to run some simple simulations for equilibrating, would you like to start trying something? Shall I give you some exercises from next class on-wards? So we will stop with this today and we will continue in next class.