Foundations of Computational Materials Modelling
Narasimhan Swaminathan
Department of Mechanical Engineering
Indian Institute of Technology Madras
LAMMPS exercises 5

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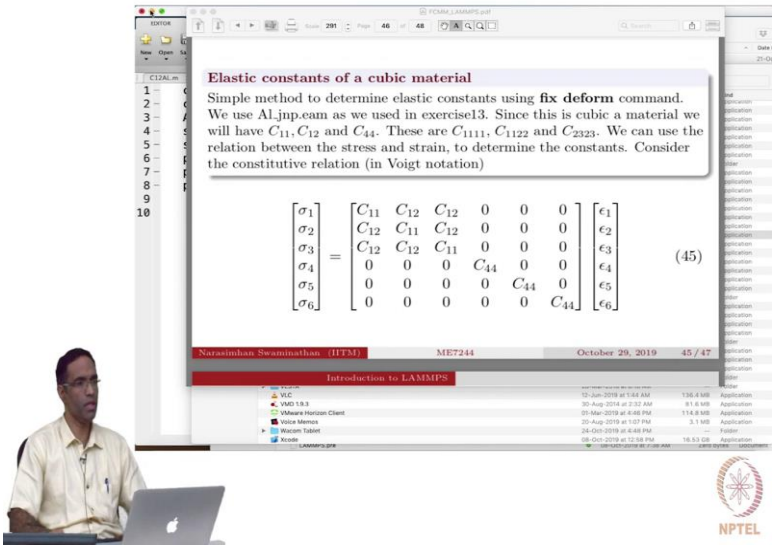

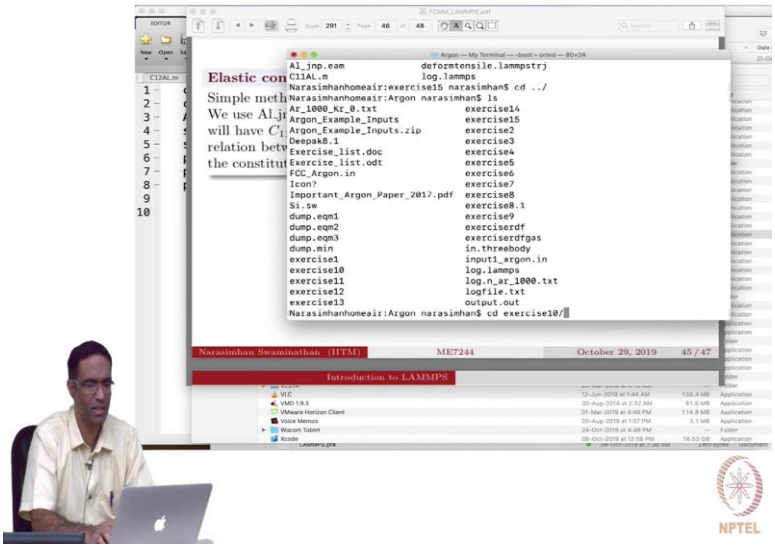

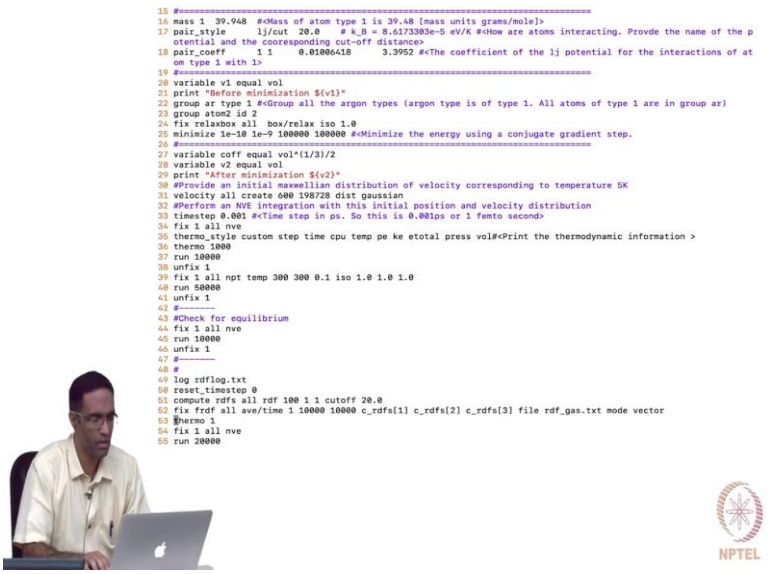

So, good afternoon. Let us continue with where we left from, where we left off. So, basically in today's class what I wanted to tell you was I wanted to clarify some of the issues concerning this the frequency with which you have to n every, n repeat, that particular issue that we had yesterday. So, I was hoping that you would have gone back and tried out what happens when you, so that was exercise number 10. So, when I basically write at the end when I used reset underscore time step 0 and then if the same understanding that we had previously, if we calculate these average time values then this one has to be the frequency and this one has to be how, this is n every.

So, every so many inputs has to be taken amongst the 10000 different configurations and we take all the 10000 configurations in order to perform the average. So, when I did this and I looked at my rdf underscore gas dot txt, I found two sets of information like what I should

want for 20000. The next part 20000 does not basically contain the header, so you might get confused that it is not printing out the next set of information. So, it works out really fine. And I also the best thing to do if at all you have such doubts is to run it for a small period of time and manually average it to see actually see whether it is doing what you want, that is what I did for this and it seems to be working perfectly fine. So, our understanding concerning what these three, value these three values are was actually correct. So, I hope you had an opportunity to try that yesterday.

So, today what we will do is we will we saw a couple of different potentials, we can keep talking about different kinds of potentials and how to give, how to feed them into LAMMPS and how to make the input script read the information, but I thought today I will actually provide you and provide you with an input script that will essentially calculate the elastic constants of a solid. So, what we are going to do is we are going to use the same idea, same interatomic potential that we used for aluminium.

And we are going to calculate its elastic constants, and all obviously, we need to be able to check whether the calculated values are close enough or not.

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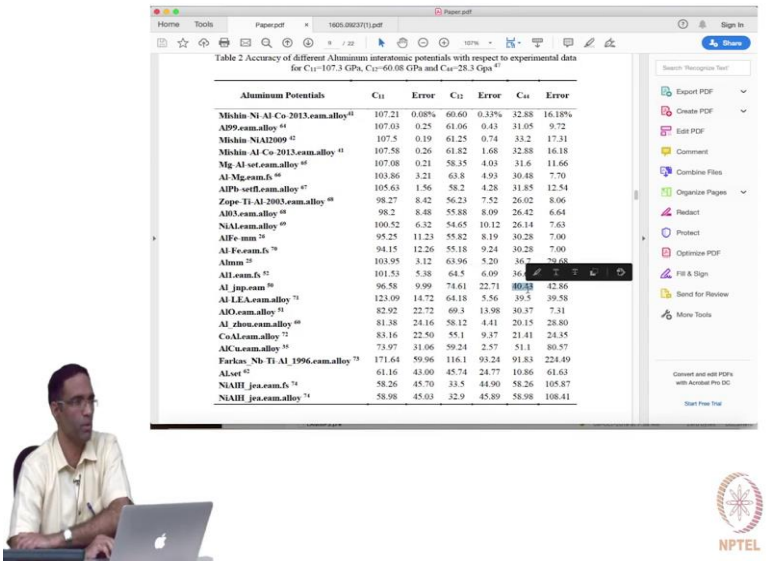

So, I am going to do some sort of a brute force method in order to calculate these elastic constants today, but it is but the methodology that we are following is quite intuitive. So, you will you will find it easy to understand. So, this will be exercise 14 and I have a paper here, where I have some document here which was got from the internet. So, I will share this with you as well and they have actually calculated the elastic constants of several metals and

alloys using embedded atom method and they have tabulated the values, so we will actually be using exactly this, if you remember right the file name that we used for the aluminium interatomic potential was also aluminium underscore jnp dot eam. And these are the values of the elastic constants that we need to calculate for this particular material.

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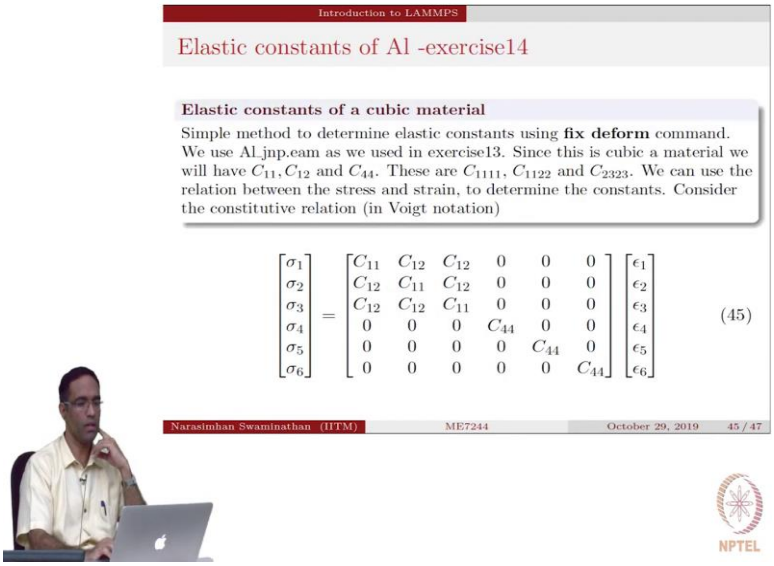

So, so, aluminium, as you might know is actually a cubic material. So, aluminium is actually a cubic metal. So, cubic metal means it will have 3 independent elastic constants basically C11, C12 and C44. So, C11, C12 and C44 are basically the elastic constants written in the voigt notation. So, I hope you know what voigt notation is, this is essentially C 1111, 1122 and 2323 if you will. So, but for the cubic material, the relationship between the stress and the strain tensor can be written as equation number 45.

$$\begin{bmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \sigma_4\\ \sigma_5\\ \sigma_6\end{bmatrix} = \begin{bmatrix}C_{11} & C_{12} & C_{12} & 0 & 0 & 0\\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0\\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0\\ 0 & 0 & 0 & C_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & C_{44} & 0\\ 0 & 0 & 0 & 0 & 0 & C_{44}\end{bmatrix} \begin{bmatrix}\epsilon_1\\ \epsilon_2\\ \epsilon_3\\ \epsilon_4\\ \epsilon_5\\ \epsilon_6\end{bmatrix} \quad (45)$$

So, you see that C11, C22 and C33 are equal C12 and C13 are all, all these things are equal. So, this, this set, this set and then all these shared components all turn out to be equal for cubic material. So, using this constitutive relationship, we can design experiments using molecular dynamic simulations in order to determine these elastic constants.

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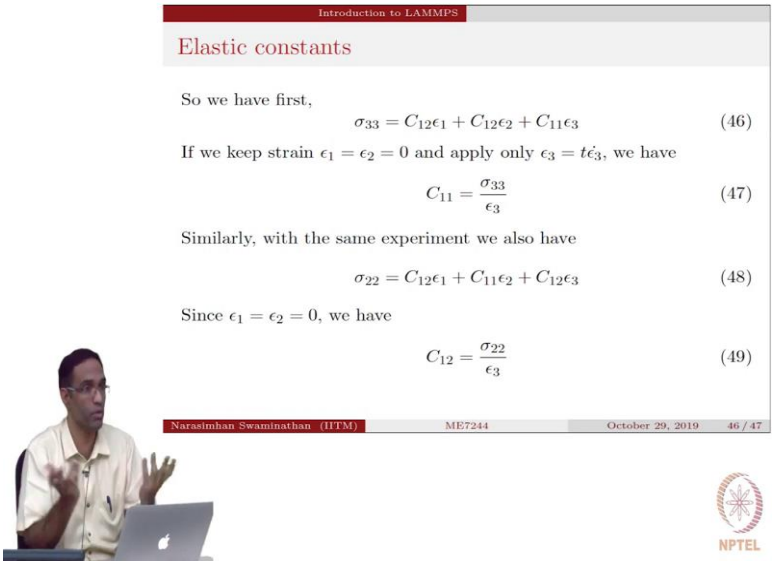

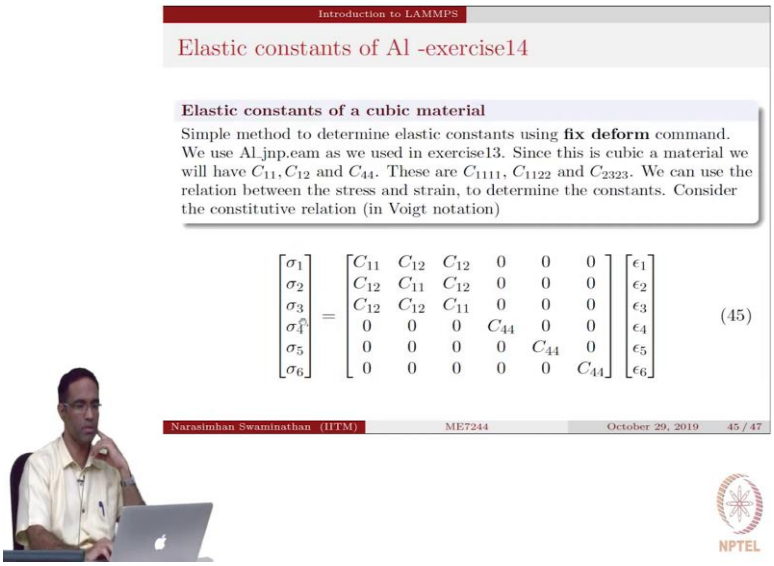

So, if you take a look at the first equation that we can write, so what what we can write for example is sigma 3 or sigma 33 is nothing but C1 2 times, C12 times epsilon 1, C12 times epsilon 2 and C11 times epsilon 3. Suppose, we keep the strains epsilon 1 and epsilon 2 to be 0. So, we constrain the box to not be expanding or contracting in that direction and apply only a strain in the is that z direction at a specific rate, then C11 is nothing but sigma 33 divided by epsilon 3 provided the stress strain relationship is linear for the amount of strain that we have actually given.

$$\sigma_{33} = C_{12}\epsilon_1 + C_{12}\epsilon_2 + C_{11}\epsilon_3$$

$$C_{11} = \frac{\sigma_{33}}{\epsilon_3}$$

So, we need to make sure that we are going to deform this simulation cell very little, not too much. If you do too much then you will have yielding and, and all that so that you can we can see all that as well. Now the same experiment, it is possible for us to say that sigma 2, with the same experiment, with basically epsilon 1 and epsilon 2 constraint with only epsilon 3 applied with the same experiment, you can also see that sigma 2 is actually equal to C12 times epsilon 1, C11 times epsilon 2, and C12 times epsilon 3. So, since epsilon 1 and epsilon 2 are 0, C12 turns out to be sigma 22 by epsilon 3. The slope of sigma 22 versus epsilon 3 will give you basically C12.

$$C_{12} = \frac{\sigma_{22}}{\epsilon_3}$$

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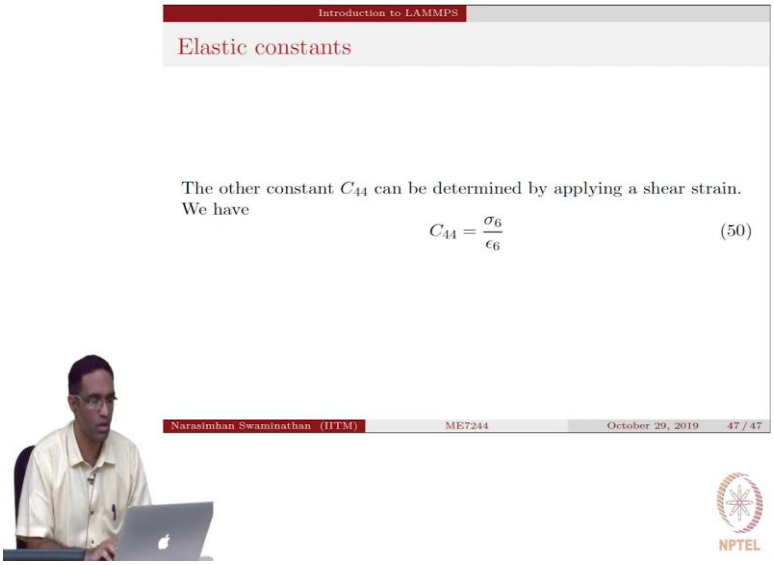

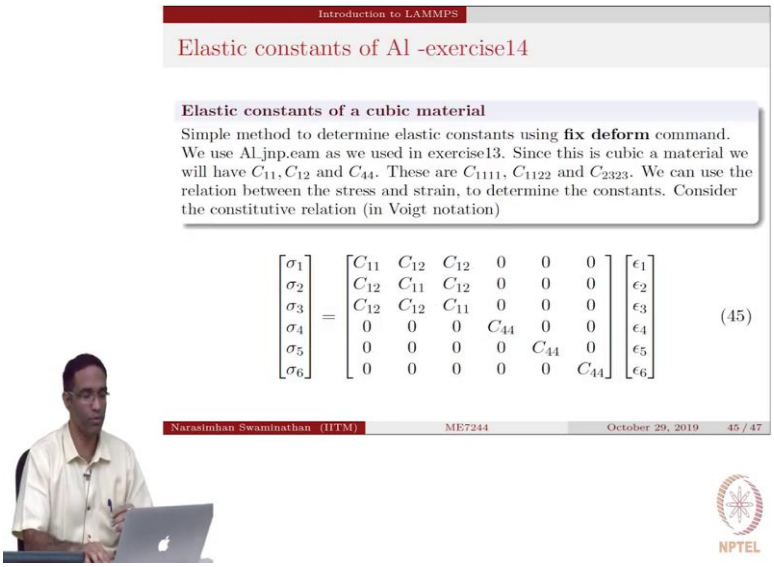

However, for the other constant C44, you need to apply a shear strength. So, sigma sigma 4 is equal to C4 times epsilon 4 or sigma 5 is equal to, sigma 5 means 2323 this is 13, sigma 13 is C44 times epsilon 13, and the sigma 12 is basically C44 times epsilon 12 or epsilon xy. So,

we can do these simple experiments in LAMMPS in order to find out these elastic constants and which is what we will be doing in exercise number 14.

$$C_{44} = \frac{\sigma_6}{\epsilon_6}$$

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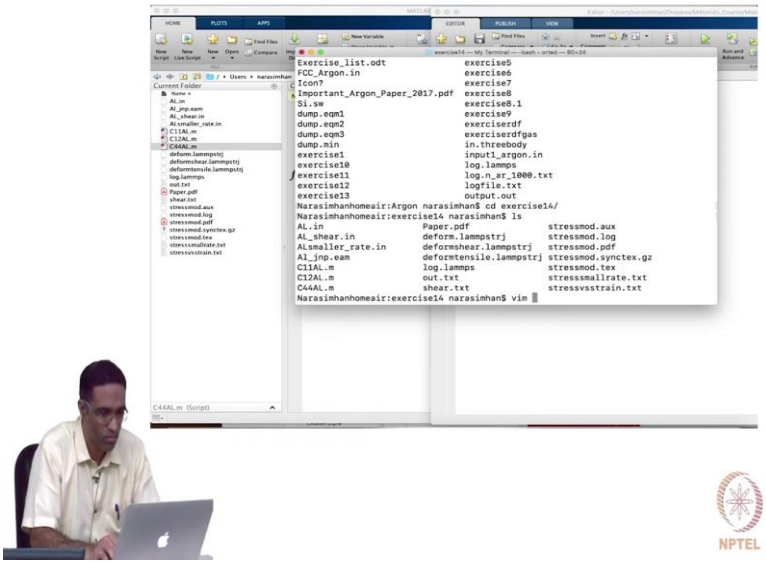

So, sigma xy, so x is one direction and y is two direction and z is three direction. So, you are asking me, why is a sigma 1 and sigma not sigma 11? Is that your question or?

Student: I am just simply asking you meaning of 1 2 3?

Professor: x y and z directions. And we have used the white notation that to voigt the equation, you know the voigt notation?

Student: Yes, sir. I am aware of it, but I do not remember it at this time.

Professor: That is fine, that is fine. So basically, it just helps you to represent a 2nd order tensor as a vector. The stress and the strain and then you are able to represent the 4th order tensor as a 2nd order as a 2 by 2 matrix, sorry, as a 6 by 6 matrix. You can you can refer to any standard books on elasticity, you will find what exactly that means, it is very simple. Now, I want to focus on writing these input scripts.

So, in this case, I am going to be deforming the simulation box in the z direction. So as before, it is a same aluminium sample with Lattice constant being 3.986, which is exactly the value that gave us the minimum energy. I have just started off with that, I just started off with that configuration, defined a region where the z direction has 20 unit cells, whereas the x and the y direction have 10 unit cells. Created in the region, created the atoms inside that region, I am saying what interatomic potential that I am going to use and then defining the file that will contain the interatomic of potential. And then I quickly minimize it, this this step might not be required in this case.

But what we want to do is we want to basically move the simulation box. So now, you imagine a simulation box, which is 10 unit cells in the x direction, 10 unit cells in the y direction and 20 units is z direction. What we want to do is I want to move the top face that is the z top face by a certain amount, by a certain amount. The command in LAMMPS which allows me to do that is basically the fix deform command. So, fix deform command is what we will be using. So first what I do is I want to compute the stress. So, I say compute stress, all pressure null virial.

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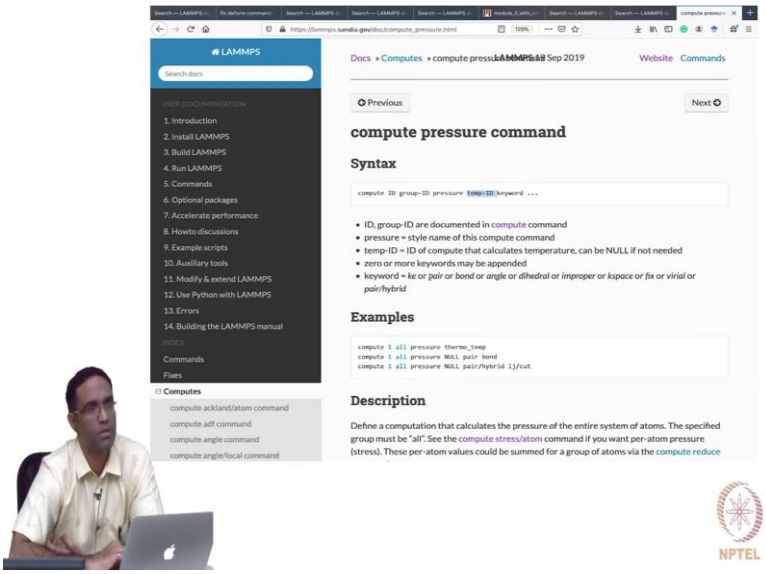

So, we will take a look at what that basically means. So, the compute pressure basically calculates the entire pressure tensor. So, it has an ID, it has a group ID basically the total group of atoms over which you want to calculate that and say pressure and then you can say temp ID basically the temperature ID is the, the idea of the fix which basically calculates the temperature.

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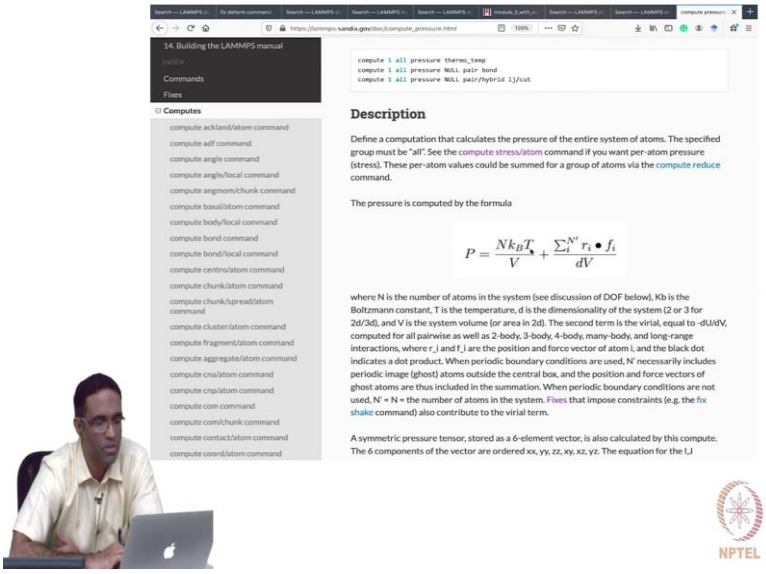

Now, the expression for stress from statistical mechanics looks something like this, it has a temperature term. And this is the other term, which basically just depends on the potential energy of the system or the forces is the temperatures f naught there will only be due to the potential energy of the system.

$$P = \frac{N k_B T}{V} + \frac{\sum_i^{N'} r_i \bullet f_i}{dV}$$

$$P_{IJ} = \frac{\sum_k^N m_k v_{kI} v_{kJ}}{V} + \frac{\sum_k^{N'} r_{kI} f_{kJ}}{V}$$

Student: Sir, the ri dot fi?

Professor: Yeah, ri dot fi.

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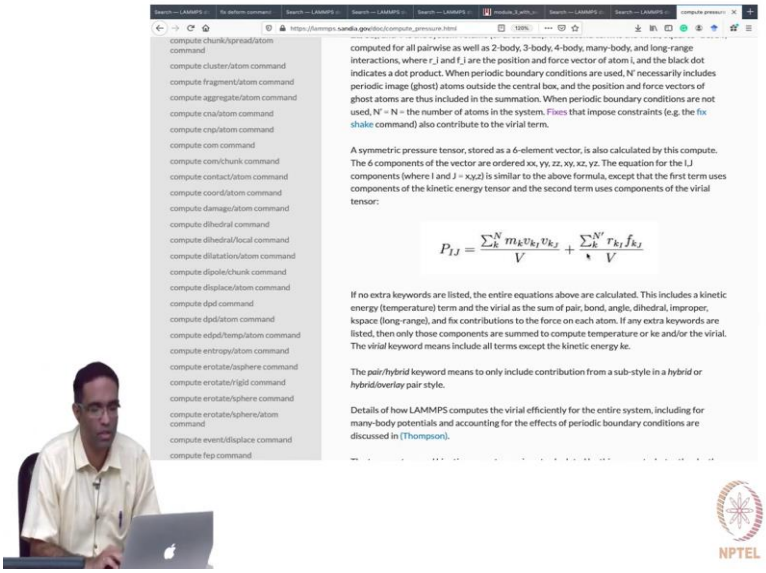

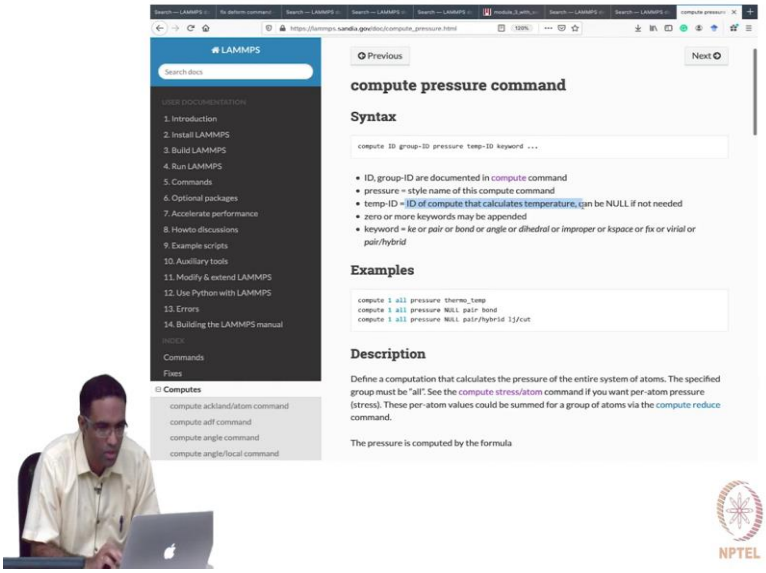

So, this is the stress configuration. And this term as you can imagine, is associated with the velocities of the atom. And these velocities are 0 when you are actually calculating the elastic constants at 0 K. I do not want to calculate the temperature effects, just for the heck of it, just to see how good our calculations are without including those terms. And as you can imagine, metals and ceramics may not show a significant deviation from in their elastic constants unless in otherwise you are going to reach really high temperatures

So, we are interested only in this term for now. So, what I have to do is, it says here give the ID of the compute that calculates the temperature and can be null if not needed. So, I am going to say null, that is why I have given in that particular keyword, the word null. And then keyword, kinetic energy or pair or bond or angle or dihedral all these things is given. I am just going to give virial. So basically, the virial component of the stress alone is considered here. So basically, the second part is going to be considered here. See all the other terms actually do not make any sense for this particular case, you can if there are dihedral angles or if there are angle potentials associated with your interatomic potential, then you would be able to calculate stress components associated only with that potential for your system. For now, we just are going to give virial.

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You could try what happens with other things, I have not tried it at this point. And then I am going to initialize the current length of the box il. And then calculate the strain to be lz minus dollar il divided by dollar initial l. So basically, the current length minus the initial length divided by the initial length would give me the strain. And then I set fix, this is the fix ID, the ID for the fix, this is the group of all the atoms over which I want to apply this fix and they set deform. And then I gave how frequently I want to deform it. So, every how many steps do I want to perform this deformation. So, I say 1 there. Can you all see this? Yes.

And then I say in the z direction and the delta by how much do I want to extend the and the z direction. So, that is given by the keyword delta. And then the first and the second terms tell me how much in the z low, do I want to increase and how much in the z high, do I want to increase the length of this simulation box. So, that is 0.0 for z low and say 1.59444, is z high. So, 1.5944 turns out to be about 2 percent strain. And then I set all these units distance units is in the box units, that means it is in angstroms.

And then I dumped all the coordinates as it is performing this deformation. And I also print out the output of the compute command using the C underscore str1 it is a array, because it is an array, it is a pressure, it is a pressure is going to be an array with 6 components, because it calculates the pressure tensor. So, the compute will have in str 6 components, this is the xx component, this is the yy, zz, xy, xz and yz components. And then I am printing a variable, which is a strain for that as it is deforming, I want to print the variable.

And I also have just plotted the x lx and ly just to show you that, that is actually not changing when I am actually performing this test. As I run this for about 10000 what, what this means is this deformation of 1.5944 will be achieved in about 10000 steps. So, if you look at this calculation carefully, this strain is about 0.02 and the strain rate is 0.02 per picosecond. So, 1234 so by not per picosecond by per 10s of picoseconds, in 10s of picoseconds because we have 10000 here. So, 10000 multiplied by 0.00 1234, so 10s of picosecond.

And this turns out to be 0.02 and 10 to the power 11 strains per second. Is that right? And that is a huge strain rate. So, I the reason why I made this simple calculation here is to show you that because of the timescales and the length scales that are actually involved in molecular dynamic simulations, whenever you perform such deformation experiments.

Student: Not the per second, it is still per picosecond.

Professor: Is it?

Student: Sir 0.02 per 10 picoseconds.

Professor: Yeah. So, which is which is 0.02 times, so 10 picoseconds is 10 into 10 to the power minus 12.

Student: Seconds.

Professor: Seconds, so, it goes the numerator and you get 100 to the power 11. So, I think this is correct. So, 2 into 10 to the power 9 strains per second, so huge strain rate. So, so, these calculations you can for, for the sake of calculating elastic constants, this might not be very important. But when you are talking about plasticity when there is deformation beyond the elastic regime, what will happen is you will, your, your stress strain plot is a very strong function of the rate at which you are actually pulling this thing, you must have studied these effects a lot in your material science.

So, whenever you are interpreting results in molecular dynamic simulations, especially those pertaining to these highs, plasticity and yielding and all that, you need to interpret your results very carefully. And if you are going to do realistic strain rates, your simulations will never complete within a reasonable time. So, you have to know how to interpret your results, at least qualitatively when you are performing these experiments. So, that is something that you need to keep in mind.

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So, when I do this, I get the, since I am plotting the, all the, the entire stress tensor and the corresponding strain in the thermo file. So, I will have the information in log file and I have actually deleted all the other lines which are not needed and I got a file which only has the stress and strain information. And the last two columns of every row is 39.86 which is lx and ly essentially not, clearly not changing, which means there is no strain in the, the other two directions.

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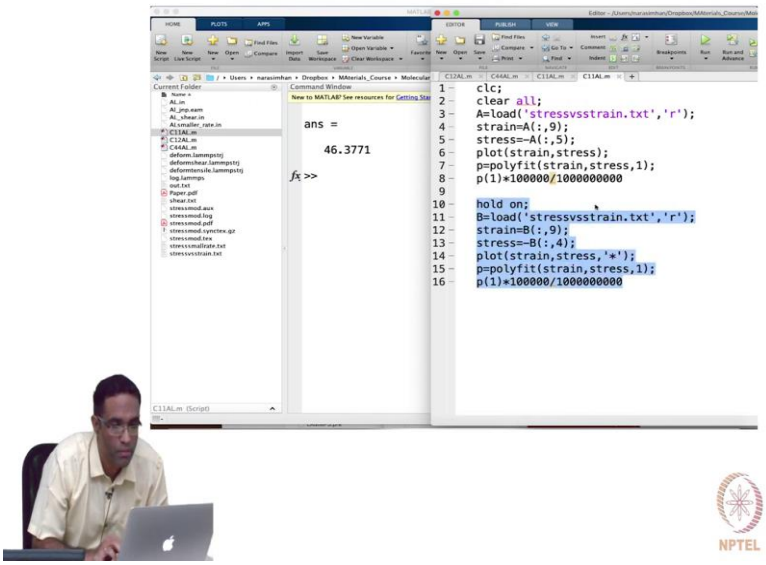

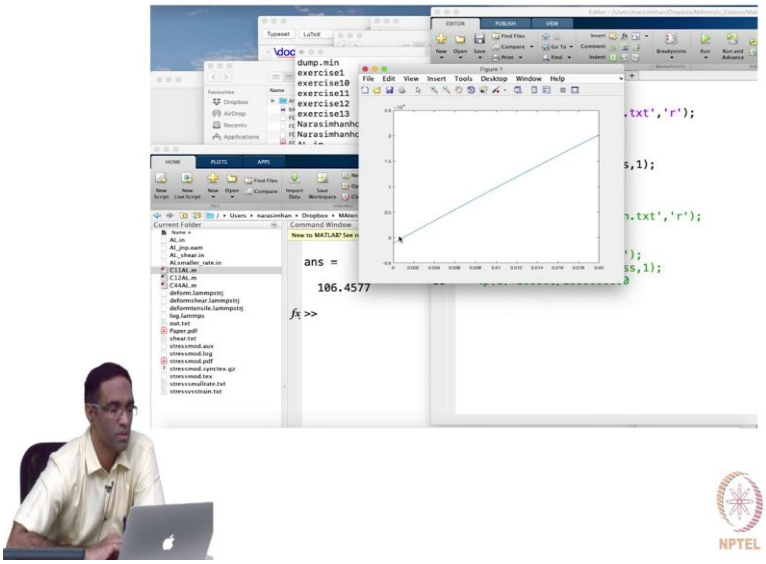

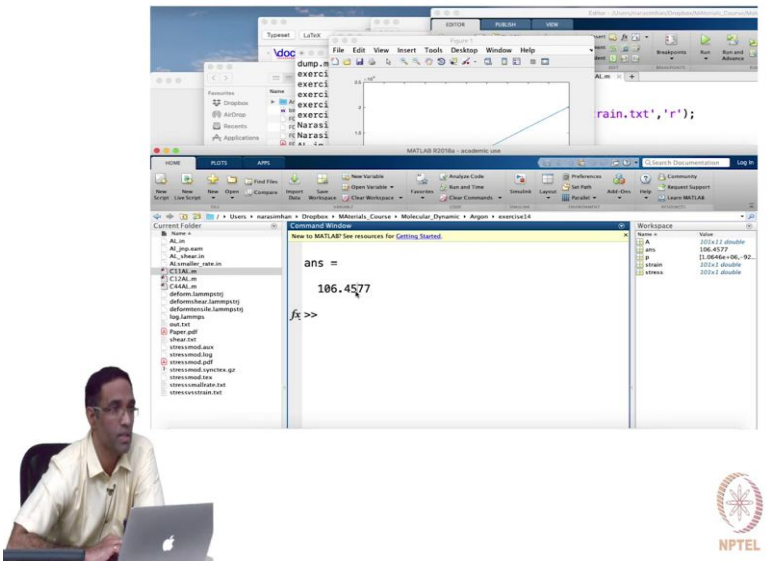

So, when I read this file and plot it, exercise 14, so I am going to first, somewhat I get a straight line however, you see that it is not really starting at 0, but there is there is a 0 stress state and a some sort of a positive strain value. So, these are some of the issues that you actually need to fix before you actually start calculating your stresses. But let us see what happens when you do this. When I did this, the slope of this line turned out to be 106.4577 gigapascals.

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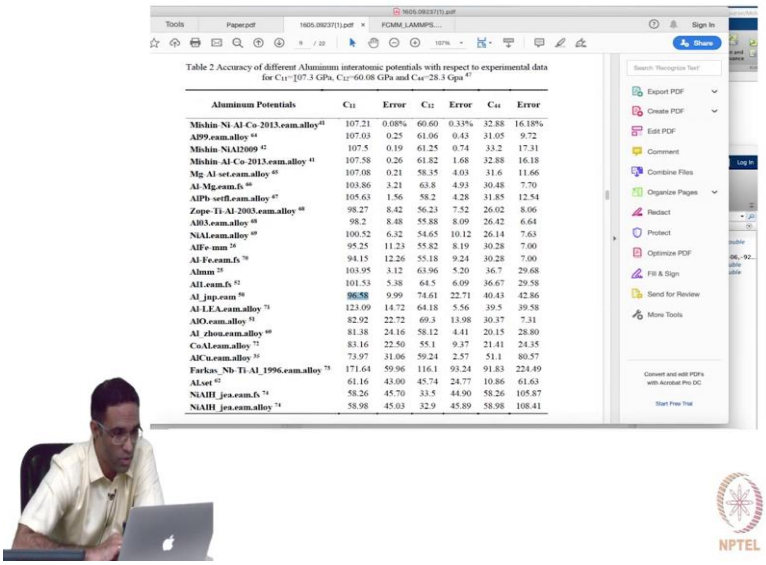

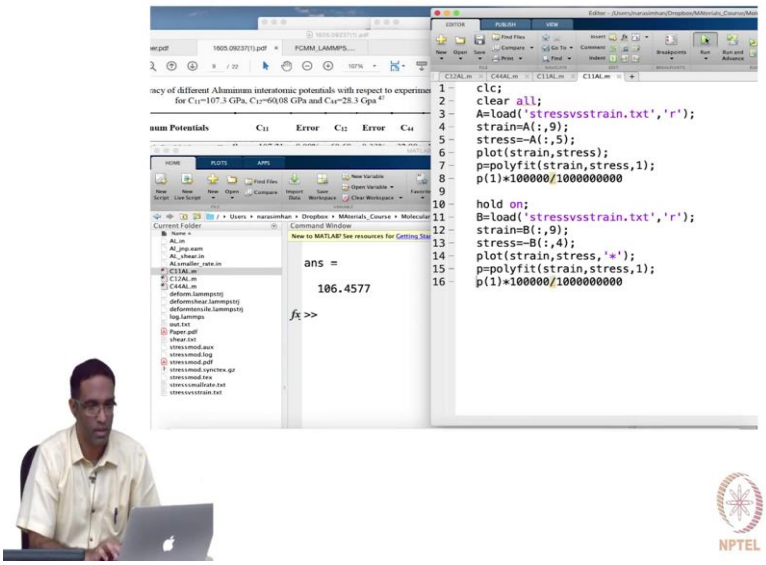

So, let us check that paper and see what values they have. This is a very crude method, this actually takes a few seconds to run, it does not even take, it is not a long simulation. It is a very very quick simulation. So so, you do not have to expect the exact value turning out here, 96.58 is the value that these guys are getting. And the actual value is 107.3 gigapascal from experiment, so we are actually closer to experiments and what this and what this paper is telling us. Now what happens to C12, the C12 is also calculated in a very similar manner except that I need to, 79.971 is what I get and according to this paper, it is 74.61. So, in this we are quite far away from the experiments but closer to this value. At least it is in the same ballpark, at least it is in the same order of magnitude. From really, really simple calculations, something that runs very, very fast. So, that is C11 and C12.

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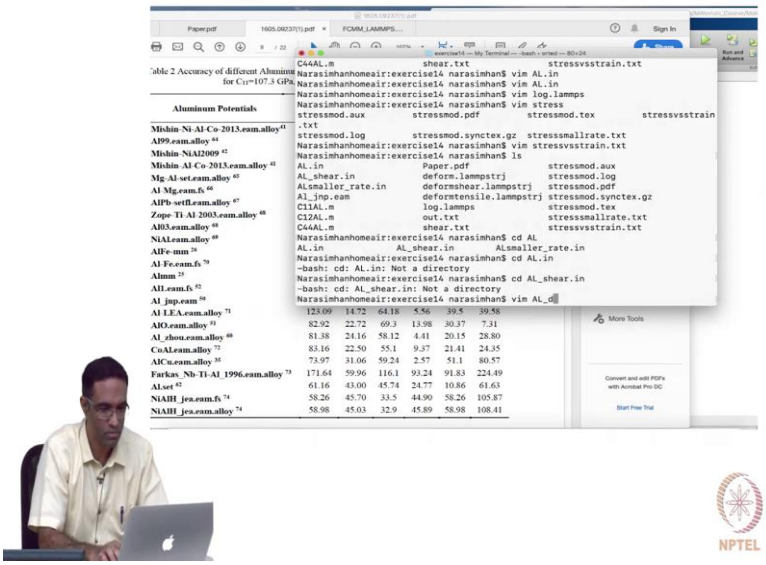

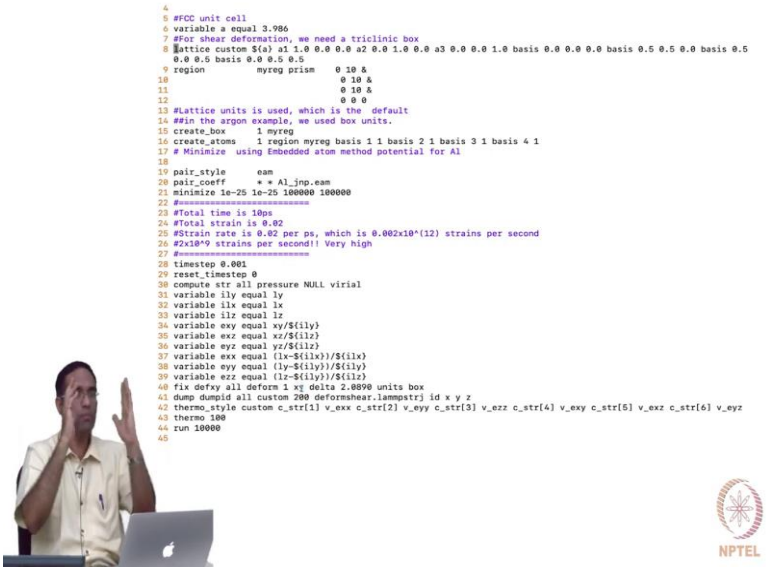

The next thing is applying shear. So, that is that in the, AL underscore. So that is the calculation that, that's needs to be done for a shear case, for a shear deformation, the same fix deform command is going to be used here. So, I am going to be talking about certain important lines and then going back here and, and tell you why I actually did it, did it this way. If you notice here, here, the Lattice structure is not defined just as Lattice FCC dollar a. I am defining it, like what I did for other crystal structures.

And that is because my, my simulation box needs to be a triclinic box if I want to be able to tilt it in LAMMPS. So, if the fixed deform command has to have a xy, so previously, we had an z here, telling that I want the z part, the z direction to be deforming for the simulation box. Now I am saying the x,y needs to be deforming. So, if that has to happen, then what I am

supposed to give you. So, imagine, imagine this to be the x axis and this to be the y axis, what I am supposed to be giving is the distance by which y needs to be moved towards x, so basically, this distance, that is what I am supposed to be giving in order to deform the simulation box and share it. So, xy means distance, y needs to be moved in the direction of x, that is what it means. xz means distance z needs to be moved in the direction of x.

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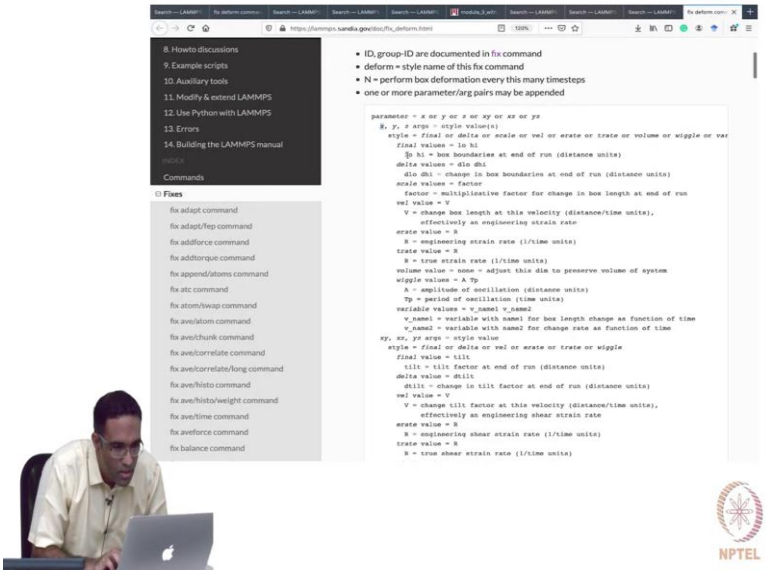

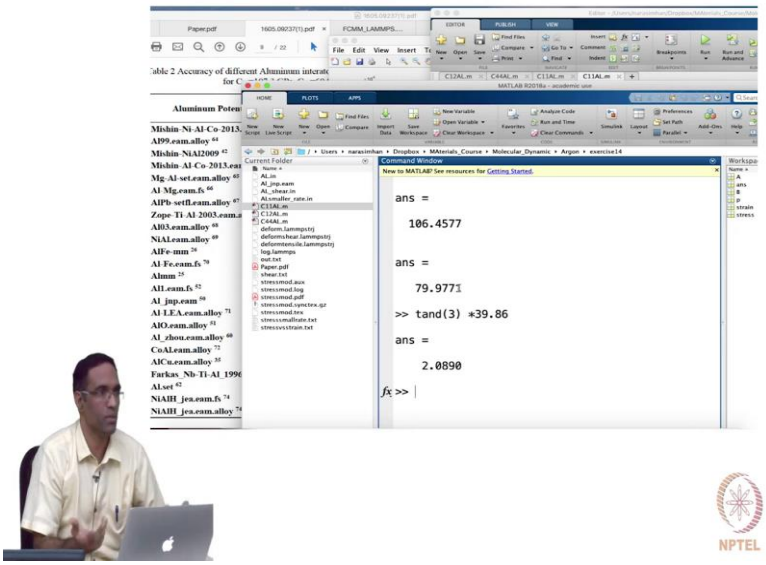

So, you will find these things in the manual. And it can be pretty confusing the first time you look at it. So, the tilt, the extent of tilt that needs to be given to these axis, is what is being given here. So, let us take a look at the fix deform command. So, the fix deform command takes an ID, a group ID, all here deform is the keyword of the style, sorry, the name of this command, n is every step and then parameter can either be x, y,z, xy, xz or yz. So, what that means is, xy means like I said, you need to give the value of the tilt, the distance, this this second thing, axis needs to be moved towards the first variable, that is important to remember.

So, how do you figure that out? So that also needs to be in angstroms. So, what you can do is, so you take your MATLAB, and then you say that say you want a 3 degree tilt. So tan d 3 degrees multiplied by this y will actually give you this distance. So, this y turns out to be

39.86 in our case, which is 2.0890. So, so, that is the reason why I have here 2.0890 units is box again and this and, what is that?

Student: Low and high, I mean 0.

Professor: No, there is low and high there is just the total amount of tilt that you are to give for the xy, only for x y and z do you need to give a how much you want to pull, push down in the x, how much you want to pull up in the xy, how much you want to increase that. But that also you see, I gave this to be 0 and just increase this. So, it is the same thing. They are just giving you an option to do that if in case that is required. So…

Student: Sir, 0 minus this thing, will it give an error?

Professor: Yes, it gave an error. Yes, that is right. You cannot put 0 here, because delta, for example, if you see x here, Delta is d low and d high, whereas xy is just the tilt, it is just a tilt.

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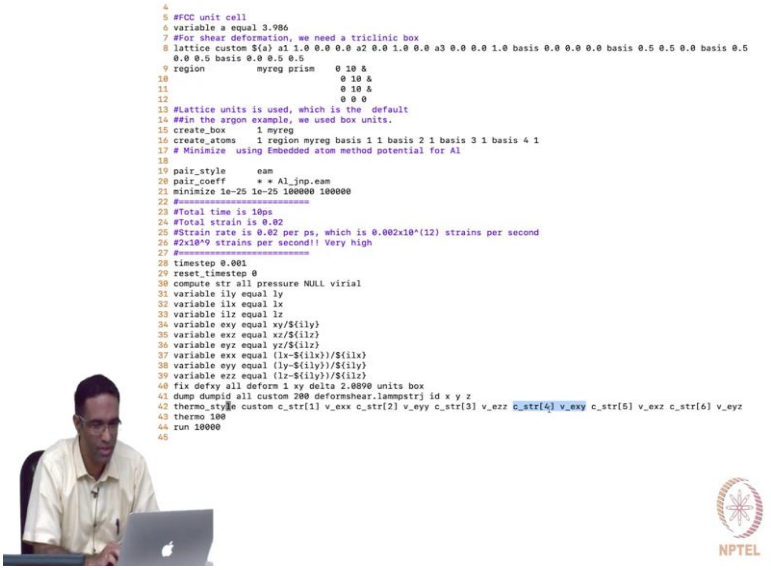


```
Narasimhanhomeair:exercise14 narasimhan$ ls
AL.in                   C44AL.m                 out.txt                 stressmod.tex
Al_shear.in             Paper.pdf               shear.txt               stresssmallrate.txt
ALsmaller_rate.in       deform.lammpstrj        stressmod.aux           stressvsstrain.txt
Al_jnp.eam              deformshear.lammpstrj   stressmod.log
C11AL.m                 deformtensile.lammpstrj stressmod.pdf
C12AL.m                 log.lammps              stressmod.synctex.gz
Narasimhanhomeair:exercise14 narasimhan$ vim log.lammps
Narasimhanhomeair:exercise14 narasimhan$ ls
AL.in                   C44AL.m                 out.txt                 stressmod.tex
Al_shear.in             Paper.pdf               shear.txt               stresssmallrate.txt
ALsmaller_rate.in       deform.lammpstrj        stressmod.aux           stressvsstrain.txt
Al_jnp.eam              deformshear.lammpstrj   stressmod.log
C11AL.m                 deformtensile.lammpstrj stressmod.pdf
C12AL.m                 log.lammps              stressmod.synctex.gz
Narasimhanhomeair:exercise14 narasimhan$ cd ../exercise15/
Narasimhanhomeair:exercise15 narasimhan$ ls
AL.in                   C11AL.m                 deformtensile.lammpstrj strain.txt
Al_jnp.eam              DELTZ.txt               log.lammps
Narasimhanhomeair:exercise15 narasimhan$ vim log.lammps
Narasimhanhomeair:exercise15 narasimhan$ cd ../
Narasimhanhomeair:Argon narasimhan$ ls
Ar_1000_Kr_0.txt            dump.min                    exercise7
Argon_Example_Inputs        exercise1                   exercise8
Argon_Example_Inputs.zip    exercise10                  exercise8.1
Deepak8.1                   exercise11                  exercise9
Exercise_list.doc           exercise12                  exerciserdf
Exercise_list.odt           exercise13                  exerciserdfgas
FCC_Argon.in                exercise14                  in.threebody
Icon?                       exercise15                  input1_argon.in
Important_Argon_Paper_2017.pdf  exercise2               log.lammps
Si.sw                       exercise3                   log.n_ar_1000.txt
dump.eqm1                   exercise4                   logfile.txt
dump.eqm2                   exercise5                   output.out
dump.eqm3                   exercise6
Narasimhanhomeair:Argon narasimhan$ cd exercise14/
Narasimhanhomeair:exercise14 narasimhan$ ls
AL.in                   C44AL.m                 out.txt                 stressmod.tex
Al_shear.in             Paper.pdf               shear.txt               stresssmallrate.txt
ALsmaller_rate.in       deform.lammpstrj        stressmod.aux           stressvsstrain.txt
Al_jnp.eam              deformshear.lammpstrj   stressmod.log
C11AL.m                 deformtensile.lammpstrj stressmod.pdf
C12AL.m                 log.lammps              stressmod.synctex.gz
Narasimhanhomeair:exercise14 narasimhan$ vim s
```

```
ALsmaller_rate.in       deform.lammpstrj        stressmod.aux           stressvsstrain.txt
Al_jnp.eam              deformshear.lammpstrj   stressmod.log
C11AL.m                 deformtensile.lammpstrj stressmod.pdf
C12AL.m                 log.lammps              stressmod.synctex.gz
Narasimhanhomeair:exercise14 narasimhan$ vim shear.txt
```

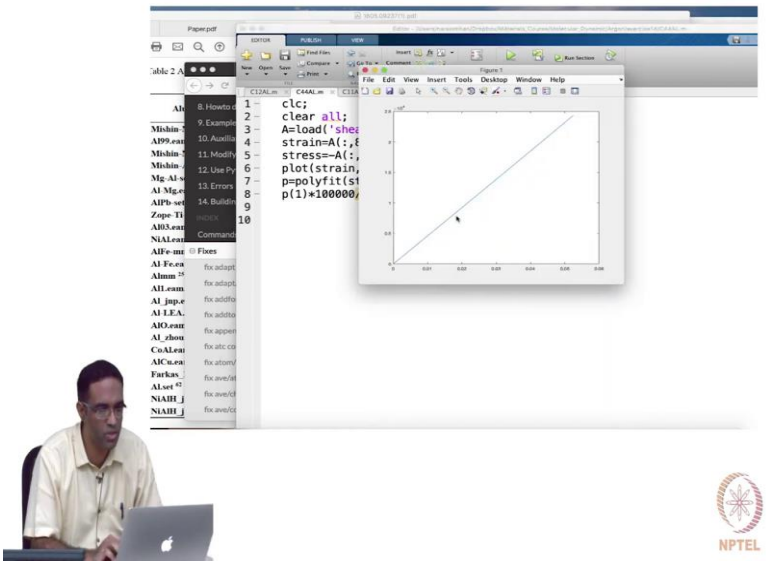
```
  1    1103.9019            0    1103.9019            0    1103.9019            0 -6.2877096e-11            0 4.756
9212e-11            0 4.5697901e-12            0
  2    1104.0913            0    1104.3042            0    1103.8595            0   -239.38655 0.0005240843 3.68918
57e-11            0 2.8089323e-11            0
  3    1104.667            0    1105.5275            0    1103.7307            0   -481.19715 0.0010481686 -2.4309
486e-12            0 2.1724489e-11            0
  4    1105.6376            0    1107.5802            0    1103.5154            0   -723.01136 0.0015722529 -2.8038
064e-11            0 2.6144635e-11            0
  5    1107.0437            0    1110.503            0    1103.2136            0   -964.79458 0.0020963372 1.94549
62e-11            0 1.7932986e-11            0
  6    1108.8857            0    1114.296            0    1102.8253            0   -1206.5527 0.0026204215 -1.5221
165e-11            0 1.8430484e-11            0
  7    1111.1634            0    1118.9592            0    1102.3506            0   -1448.2916 0.0031445058 2.14554
74e-11            0 2.2290015e-11            0
  8    1113.8772            0    1124.4928            0    1101.7894            0   -1690.0173 0.0036685901 2.01209
8e-11            0 2.6286426e-11            0
  9    1117.027            0    1130.8968            0    1101.1418            0   -1931.7358 0.0041926744 -2.8673
537e-12            0 1.9294865e-11            0
 10    1120.6111            0    1138.1697            0    1100.4072            0   -2173.4515 0.0047167587 3.80613
38e-11            0 2.4699898e-11            0
 11    1124.6288            0    1146.3107            0    1099.5852            0   -2415.1697  0.005240843 -1.3522
239e-11            0 1.8574427e-11            0
 12    1129.0815            0    1155.3214            0    1098.6766            0   -2656.8951 0.0057649272 9.92883
11e-12            0 -1.3418668e-12            0
 13    1133.9698            0    1165.2025            0    1097.6815            0   -2898.6332 0.0062890115 1.69397
51e-11            0 2.1728973e-11            0
 14    1139.2939            0    1175.9543            0    1096.5999            0   -3140.3897 0.0068130958 -8.5139
375e-13            0 2.9326214e-11            0
 15    1145.0539            0    1187.5771            0    1095.4319            0   -3382.1704 0.0073371801 -1.1507
684e-11            0 3.0987222e-12            0
 16    1151.2498            0    1200.0712            0    1094.1775            0   -3623.9811 0.0078612644 -2.7623
778e-12            0 -8.1101838e-14            0
 17    1157.8814            0    1213.4366            0    1092.8367            0   -3865.8278 0.0083853487 1.69207
93e-11            0 1.5840488e-11            0
 18    1164.9487            0    1227.6735            0    1091.4091            0   -4107.7164  0.008989433 -2.5734
912e-13            0 -3.958191e-12            0
 19    1172.4514            0    1242.7819            0    1089.8946            0   -4349.6527 0.0094335173 -1.0851
496e-11            0 1.1322659e-11            0
```

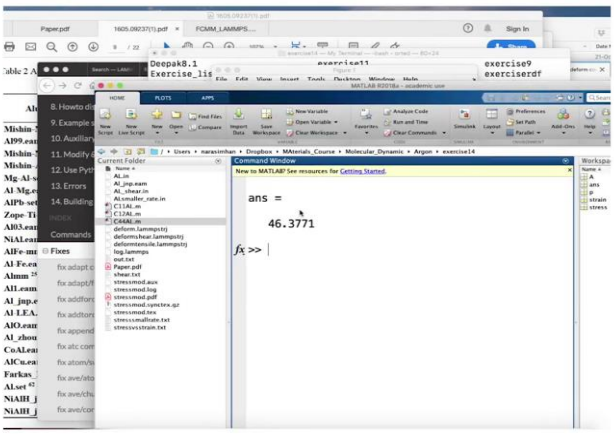
```
 81    2455.7413            0    3857.6157            0    827.63164            0   -19411.531  0.041926744 -1.1008
433e-12            0 1.8816194e-12            0
 82    2489.6489            0    3927.114            0    820.70253            0   -19656.207  0.042450828 -1.8114
499e-12            0 7.1173007e-12            0
 83    2523.9258            0    3997.4389            0    813.68852            0   -19900.944  0.042974912 1.35250
48e-11            0 8.5978481e-12            0
 84    2558.5731            0    4068.592            0    806.58939            0   -20145.751  0.043498996 1.50747
6e-11            0 4.3405282e-12            0
 85    2593.6283            0    4140.6086            0    799.40519            0   -20390.597  0.044023081 6.30206
92e-12            0 4.8712011e-12            0
 86    2629.1002            0    4213.4976            0    792.13598            0    -20635.48  0.044547165 -4.7116
306e-13            0 1.4850944e-11            0
 87    2664.9888            0    4287.2599            0    784.7818            0   -20880.405  0.045071249 2.55312
8e-12            0 1.0124564e-11            0
 88    2701.2941            0    4361.8966            0    777.3427            0    -21125.38  0.045595334 2.90334
05e-12            0 1.2929775e-11            0
 89    2738.0163            0    4437.4078            0    769.81766            0   -21370.409  0.046119418 1.24213
96e-11            0 5.1008141e-12            0
 90    2775.1553            0    4513.7953            0    762.20739            0   -21615.499  0.046643502 8.35945
79e-12            0 -6.2867482e-12            0
 91    2812.7111            0    4591.0606            0    754.5125            0   -21860.655  0.047167587 8.83167
42e-13            0  1.25757e-11            0
 92    2850.6836            0    4669.2045            0    746.73309            0   -22105.883  0.047691671 1.40897
77e-11            0 2.1278349e-11            0
 93    2889.0725            0    4748.2278            0    738.86919            0   -22351.188  0.048215755 -1.0286
592e-11            0 3.4517083e-11            0
 94    2927.8776            0    4828.1314            0    730.92087            0   -22596.577  0.048739839 -1.6992
766e-13            0 5.8881748e-12            0
 95    2967.0992            0    4908.9167            0    722.88817            0   -22842.055  0.049263924 1.32708
59e-11            0 7.9455225e-12            0
 96    3006.7375            0    4990.5856            0    714.77138            0   -23087.628  0.049788008 -5.3623
763e-12            0 3.2386141e-11            0
 97    3046.7925            0    5073.1399            0    706.57073            0    -23333.3  0.050312092 -1.3620
545e-11            0 4.615783e-12            0
 98    3087.2634            0    5156.5805            0    698.28611            0   -23579.077  0.050836177 1.19370
67e-12            0 3.549206e-11            0
 99    3128.149            0    5240.9082            0    689.91729            0   -23824.965  0.051360261 2.59922
61e-11            0 2.0884993e-11            0
100    3169.4503            0    5326.1244            0    681.4646            0   -24070.969  0.051884345 -1.5636
856e-11            0 2.9448569e-11            0
101    3211.1672            0    5412.23            0    672.92813            0   -24317.095   0.05240843 1.20373
03e-11            0 1.0935933e-11            0
~
```

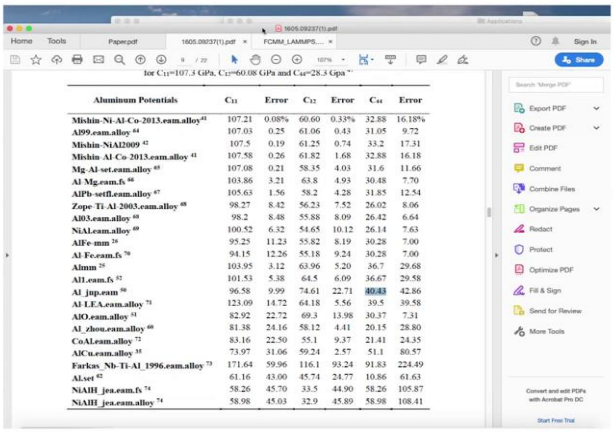
Again, this also is done over 10000 time steps. So, it will do it in about 10 Pico seconds. And I am printing out everything here. So, I am printing out the stress, the epsilon xx stress, epsilon yy, epsilon, sigma zz and the strain in the zz direction and all the correspondence and this is what we are expecting to have non 0 values. We are expecting the xy shear stress and the corresponding shear strain to have non 0 values which are the 1 2 3 4 5 6 7th and the 8th column.

So, if you take a look at the, so 1 2 3 4 5 6 7th and 8th column, so initially the strains are small. Oh no, this is not right. . No no, it is exercise 14 only. So, I just printed out all those values into another file and deleted all the unnecessary lines. So, if you look at the this is the 1st stress 1st strain, 2nd stress 2ndstrain, 3rd stress 3rd strain, 4th stress and the corresponding value of strain initially is 0. But in the next line, if you see this becomes there is a non 0 value for these strains. And finally, you reach the require, required strain, you reach the required strain.

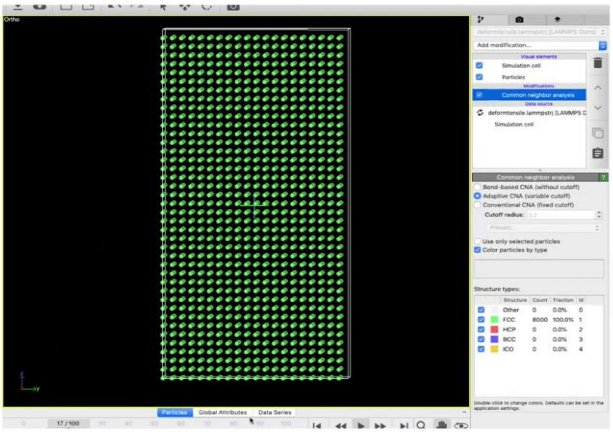
(Refer Slide Time: 27:15)

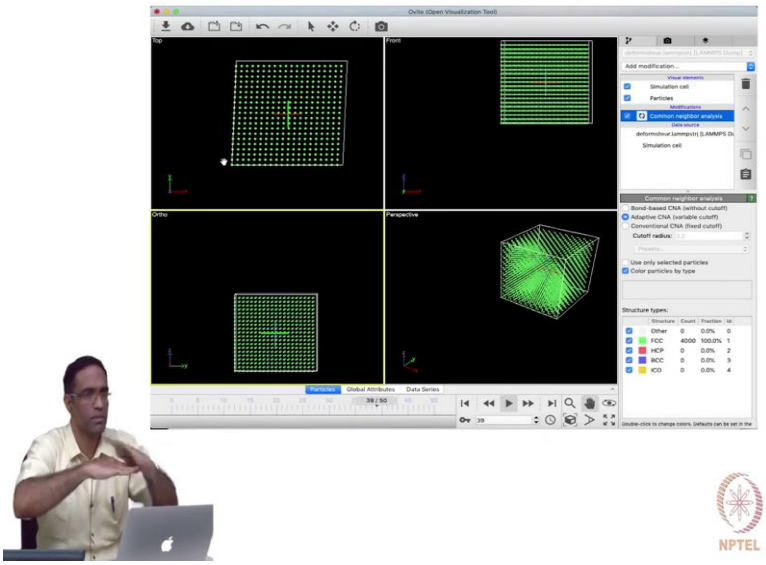






Aluminum Potentials	C_{11}	Error	C_{12}	Error	C_{44}	Error
Mishin_Ni-Al-Co-2013.eam.alloy[64]	107.21	0.08%	60.60	0.33%	32.88	16.18%
Al99.eam.alloy [64]	107.03	0.25	61.06	0.43	31.05	9.72
Mishin-NiAl2009 [42]	107.5	0.19	61.25	0.74	33.2	17.31
Mishin_Al-Co-2013.eam.alloy [41]	107.58	0.26	61.82	1.68	32.88	16.18
Mg_Al-set.eam.alloy [65]	107.08	0.21	58.35	4.03	31.6	11.66
Al-Mg.eam.fs [66]	103.86	3.21	63.8	4.93	30.48	7.70
AlPb-setfl.eam.alloy [67]	105.63	1.56	58.2	4.28	31.85	12.54
Zope-Ti-Al_2003.eam.alloy [68]	98.27	8.42	56.23	7.52	26.02	8.06
Al03.eam.alloy [65]	98.2	8.48	55.88	8.09	26.42	6.64
NiAl.eam.alloy [69]	100.52	6.32	54.65	10.12	26.14	7.63
AlFe-mm [26]	95.25	11.23	55.82	8.19	30.28	7.00
Al-Fe.eam.fs [70]	94.15	12.26	55.18	9.24	30.28	7.00
Almm [25]	103.95	3.12	63.96	5.20	36.7	29.68
Al1.eam.fs [62]	101.53	5.38	64.5	6.09	36.67	29.58
Al_jnp.eam [50]	96.58	9.99	74.61	22.71	40.43	42.86
Al-LEA.eam.alloy [71]	123.09	14.72	64.18	5.56	39.5	39.58
AlO.eam.alloy [71]	82.92	22.72	69.3	13.98	30.37	7.31
Al_zhou.eam.alloy [60]	81.38	24.16	58.12	4.41	20.15	28.80
CoAl.eam.alloy [72]	83.16	22.50	55.1	9.37	21.41	24.35
AlCu.eam.alloy [35]	73.97	31.06	59.24	2.57	51.1	80.57
Farkas_Nb-Ti-Al_1996.eam.alloy [73]	171.64	59.96	116.1	93.24	91.83	224.49
Al.set [62]	61.16	43.00	45.74	24.77	10.86	61.63
NiAlH_jea.eam.fs [74]	58.26	45.70	33.5	44.90	58.26	105.87
NiAlH_jea.eam.alloy [74]	58.98	45.03	32.9	45.89	58.98	108.41





Again, if you plot this you get a straight line. So that is C11, C12 and this is just C44. And then if you look at the corresponding value of p1, it turns out to be 46.3771. Let us see how we are doing here, 40.43, the actual value is about 28.3. So, it is not it is not great, but it is okay as far as the potential is concerned. So, this potential is supposed to not do anything better than that. So so, you need to keep in mind what experiments are saying about your values and what this potential is capable of predicting. Now, this is not a very amazing thing, because most likely these embedded atom potentials are going to be fitted for actually reproducing some of these elastic constants.

So, but in case you have an interatomic potential for which you do not know the elastic constants to get the order of magnitude, you can do some simple tests like this to actually figure it out. And you have to make sure and you are you are making sure every time that the, you are looking only in the linear portion of the curve because when you are pulling, if you look at the extent of pulling that is going on here. I will show this to you later, you can actually hardly see it being moved, it is actually being pulled off. So, it is being pulled very little, so you cannot see it much. There is some little bit of moment if you observe very carefully.

Can you see the box move? Moved a little bit. No no, wait, once it loads completely it will appear to be a little bit fast. So it is more. Oh, I should switch this off, one minute. Now I think you should be able to see it move a little bit. And the shear thing also moves very little, but that is a little bit more can be seen a little bit more clearly. You can see the box being sheared in the xy, the y is moved, like what, what expected the (extend) extend, xy specifies

how much y is moved towards x. So, you see that, it is that axis which is moving towards y by this, by this amount. This information as to what xy, yz and xz means is also useful for constructing triclinic simulation boxes. So, we have not done that, but with that information, you should be able to do it pretty easily.

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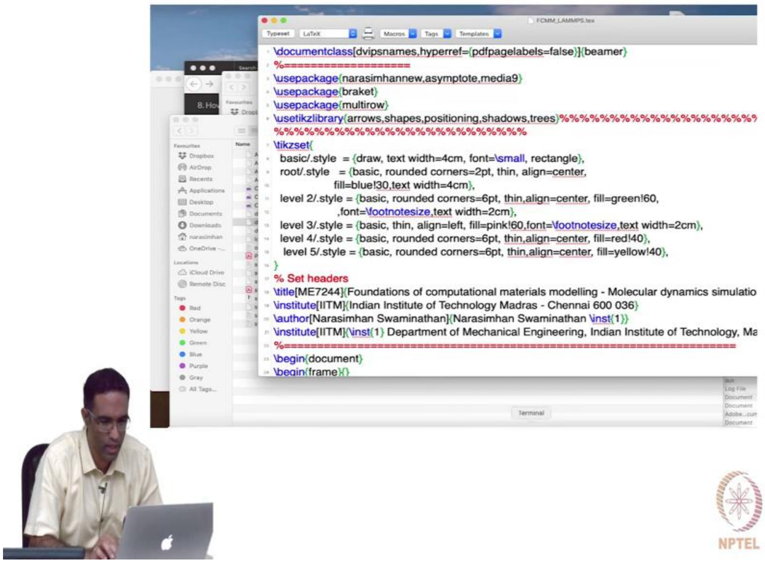
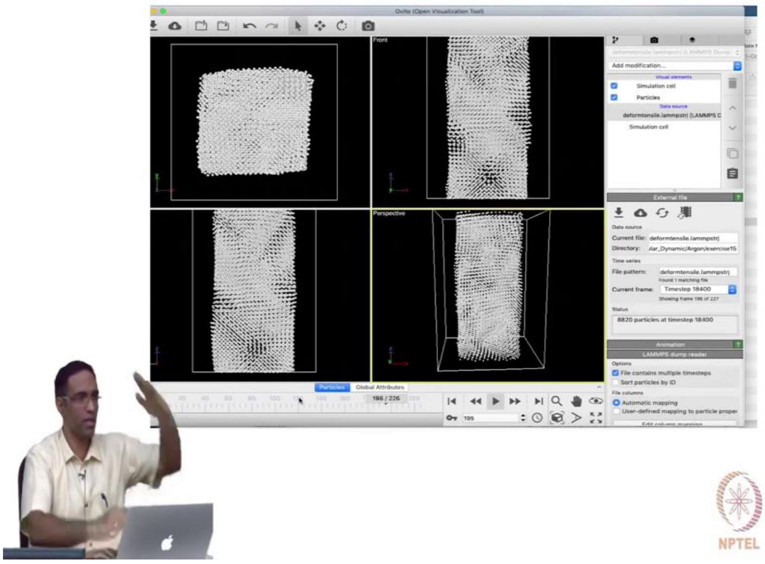
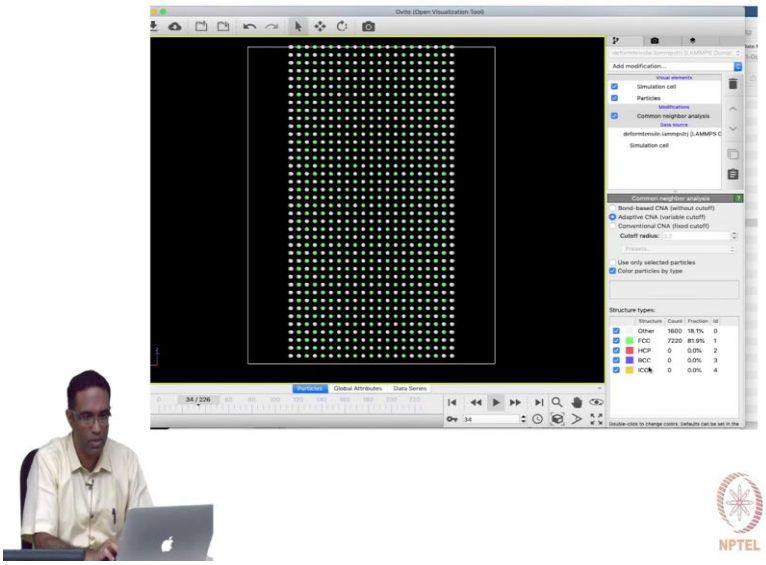
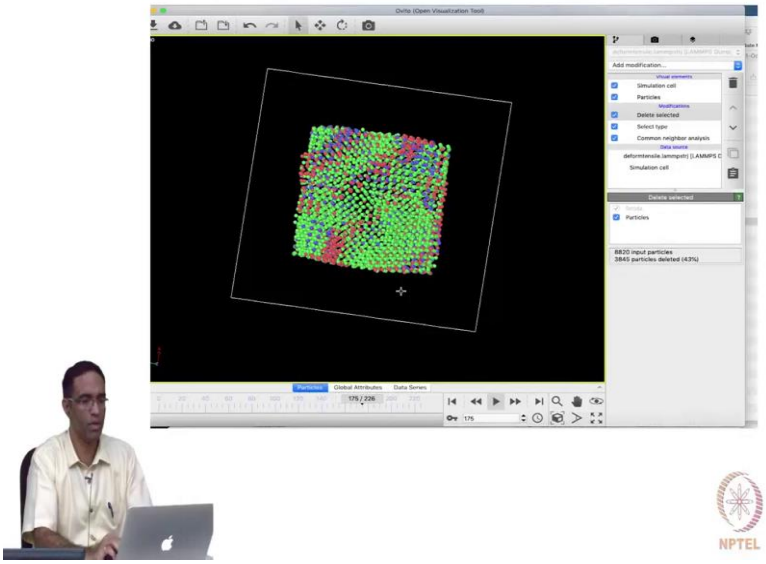








Now, what happens if you actually pull it even more? So how do we actually, I am going to exercise 15 here, I will tell you what it does. Let us look at this, so the idea is to have a long nano size or not nano some, some material with free surface. So, this is the same copper material, except that now I have an outer simulation box and an inner region in which I am actually filling the atoms.

So, I am not filling the entire region with atoms but something else. So, simulation box is the outer part and then there is another region within it, into which the atoms are being filled. And now if I, if you keep looking at it, it is being pulled. And it is not just being pulled, after every bit of pull, it is being, energy is being minimized, the energy is being minimized because we are continuously pull it, the pull rate is so fast that the atoms are not going to occupy their minimum energy positions unless I actually minimize it for every step of

pulling. So, you see that when you look at the deformation at some particular point of time, it is, it is okay, but then all of a sudden you have the shearing shear bands, and all those things will start appearing.

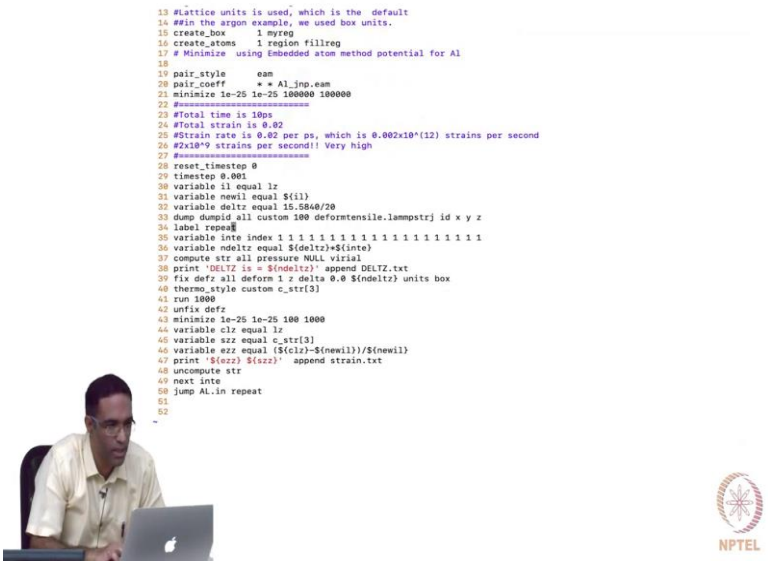
So, in order to look at this a little bit more clearly, so what is basically happening is that you are, the slip. You have studied in material science. That is going to be slip. So, you can see those slip bands somewhat. I will I will take a look at this input file in a second, but if you do something called as the common neighbour analysis, so, common neighbour analysis is a technique which is capable of identifying atoms belonging to a FCC or a HCP or a BCC or icosahedral Lattice.

So, if you just say, perform common neighbour analysis, it is basically going to colour the atoms depending upon whether they are a part of the FCC, HCP BCC, icosahedral or other, something else. So, if you take a look at this, everything else that is not in the centre is marked as other because they are atoms belonging to the free surface. So, they will not be FCC or BCC, they will relax in a slightly different way.

So, if you continue to keep looking at the colours, all of a sudden you start, some BCC atoms begin to appear and then you have some failure. So you can actually look at this, a little bit better if you do select type, select the other atoms, that is the outer shell atoms and basically delete them. So, where is this? Delete selected. And then look at only what is happening to the FCC structure. So, initially everything inside is FCC for a particular value of strain. This is again a very simple calculation, very simple small input script and you have the deformation. You have all sorts of shear bands and other things happening.

So, you see that 45 degree plane here that is over which it is actually slipping, so you can see whatever you study in your book, you can actually see it happen when you actually simulate these simple things with little apps. You can do a better job. I need to play with the input file a little bit more. But let me show you what the input file looks like. Because this time, it is just not enough if you just continuously pull it, because you have to allow these atoms as you, previously we just pulled it a little bit, so it did not really matter, we were within the elastic regime. But now we are going beyond that. So, for every pull, you might want to make sure that the atoms are reaching their equilibrium positions for that stretch. Only then we will you be able to capture this phenomenon. If you continuously pull you do not see that.

(Refer Slide Time: 34:32)



So so again, I started off with start off with a sort of FCC structure and everything, so all the same, everything is pretty much same. But what I do here is I have introduced a couple of new things here, what do I want to do, I want to be able to apply some strain to the top face, minimize the energy, apply a little bit more, minimize the energy, apply a little bit more, minimize the energy until some finite strain is reached. So, right now I am applying a total strain of 15.5840 divided by 79.72, whatever that is, I think that is a 20 percent strain. And I am saying that the amount by which I want to extend my delta are of my simulation box in the z direction is 15.580 divided by 20. So, I define a new variable which is this delta z times 1.

So, initially it is it is 15.5840 divided by 20 times 1 and I calculate a new variable n delta z and apply that to my fix all deform command. This label repeat is actually a label in the input script, so that I can use this jump command to go back here and re-repeat it for the next one and it will add it to the to the actual value that it had reached previously. So, if if lz was actually the first length and in the first step it did lz plus delta z. The second step when it comes it has to do lz plus 2 delta z to lz plus 3 delta z. So, there is a reason all this is 1 because I always have to add the same amount to the final length. So, this could be actually modified and made a little bit simpler obviously.

So, and I, I try to achieve each deformation. So, each delta z is achieved in about 1000 steps. Following that, I minimize the command and I make sure that I unfix it because next time when it go, when it when it goes back to the same, when it goes back to the loop it will find a

fix which was already defined unless I unfixed it, it is going to give me an error. So, I unfixed the deformation. So, I do this achieve a small delta z in 1000 steps minimize the energy, minimize the energy, minimize the energy for about 20 steps, in about 20 steps, I will reach 15.5840 total delta z and if you look at the I have to see if my strain (calculation) and then, sorry simultaneously I print the strain and the stress and append it to a text called strain dot txt. So, as is when it is calculating the stress and the strain it is going to fill it up with this line.

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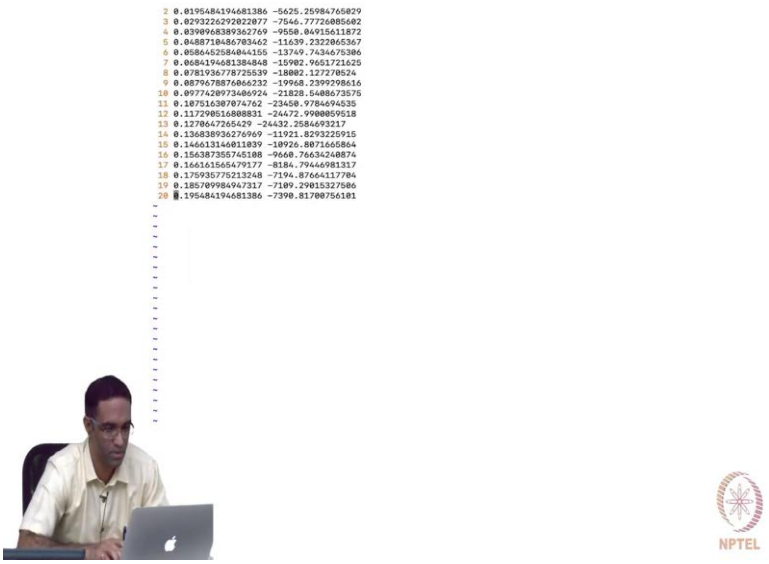

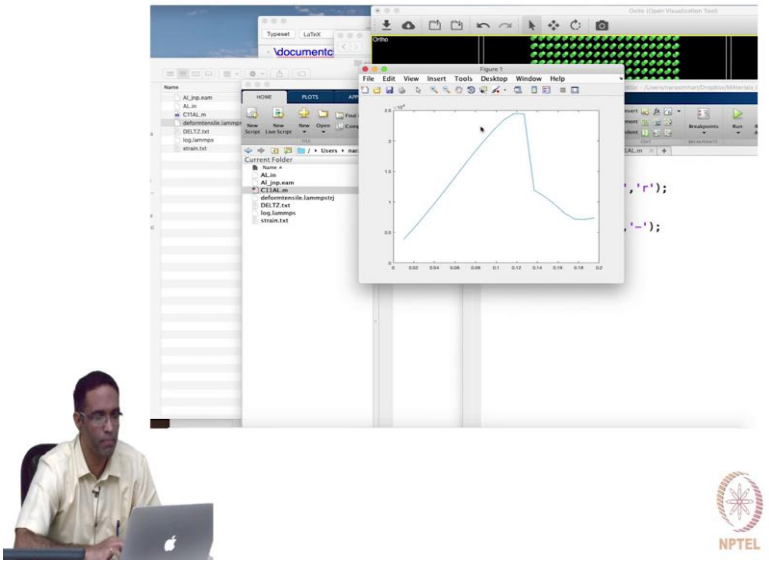

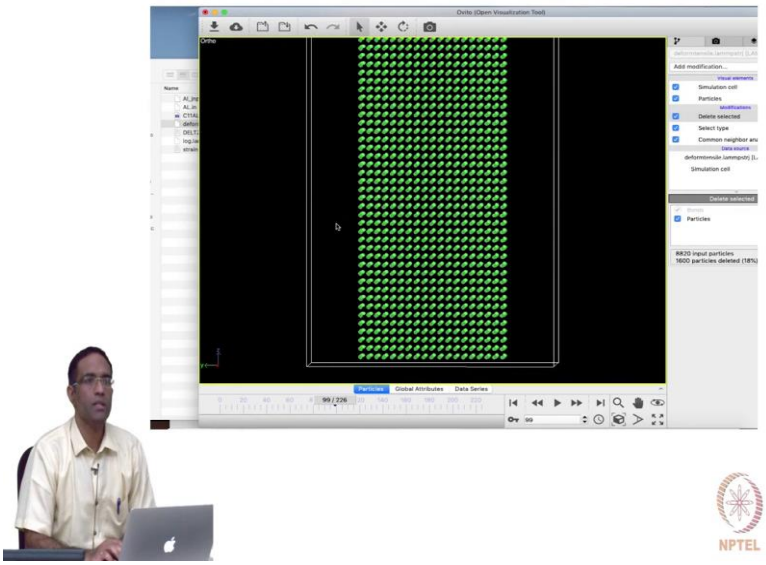

So, let us see whether this, yeah so, it contains about 20 steps about 20 steps and if we actually plot it you will see some non-linearity occurring obviously. So, it is just going up, is failing and just fail here, something has happened at this point. Until about in this case until about 10 percent strain, you are not seeing much of yeilding, which is, is that usual? No, it is not usual. You are looking at, this happening because it is not the bulk material number one, number two, it is a single crystal copper, single crystals are extremely strong, they have very high and then you are also pulling it at a very high rate no matter what you do. So, all these things are contributing to this sort of a behaviour, but you can see some failure actually happened when you brought the stress was a strain diagram.

So, these are some simple techniques that you can use in order to study the elastic properties of the materials. Now, these are extremely crude ways. Now you can, there are more elegant ways by which you can actually define the elastic constants itself as a function of the velocities and positions of all the atoms in the system and calculate it using statistical mechanics. So, once you know that you have to print out the positions and the velocities and then explicitly use that expression to evaluate your elastic constants of the material. So, anything else? Any other questions?

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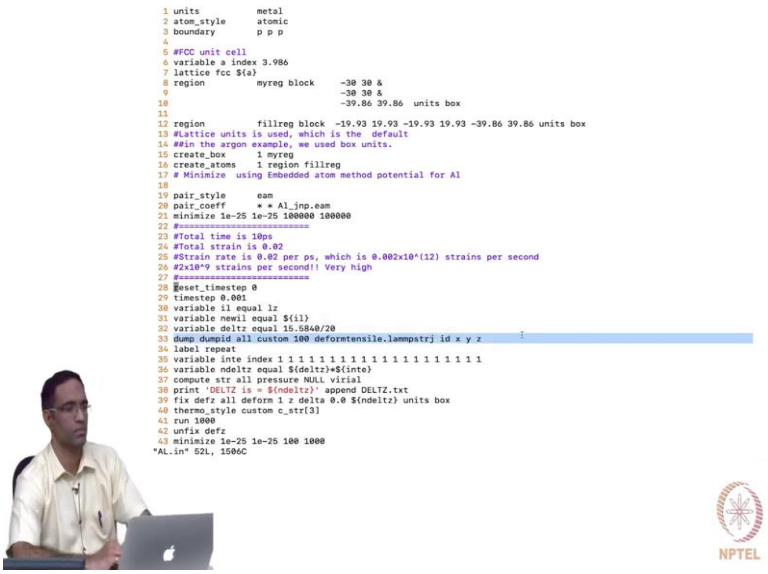

Student: can you go to line 33?

Professor: There is a dump here.

Student: So, LAAMPS trj is something that would something represent?

Professor: No, it recognizes as soon as it sees the format, that is just if you use VMD then you would have to give that, so I just I just gave it, you do not have to give it.

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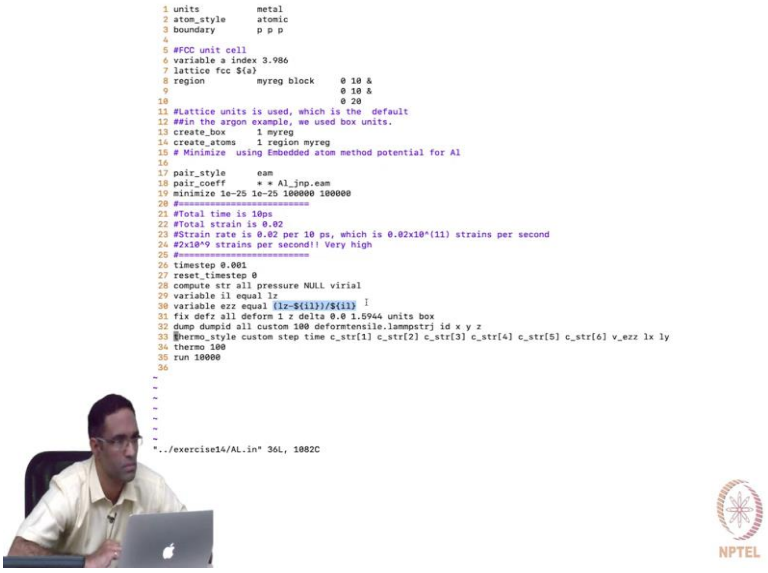

Student: Sir, can you please go to exercise 14?

Professor: The shear or the normal?

Student: Normal. where you are printing a...

Professor: Yeah yeah.

Student: Those are Lattice constants; those are elastic constant.

Professor: Which? No, they are the stresses. So, this so this is a compute right.

Student: first we are ...

Professor: This is thermo style, custom means whatever I want to print I will print. Step is the step number, time is a time it is that is taken. C underscore str1 is taken from.

Student: Those are normal stresses, first 3.

Professor: First 3 are normal stresses, this next 3 are shear stresses and then this is the strain that I calculate here.

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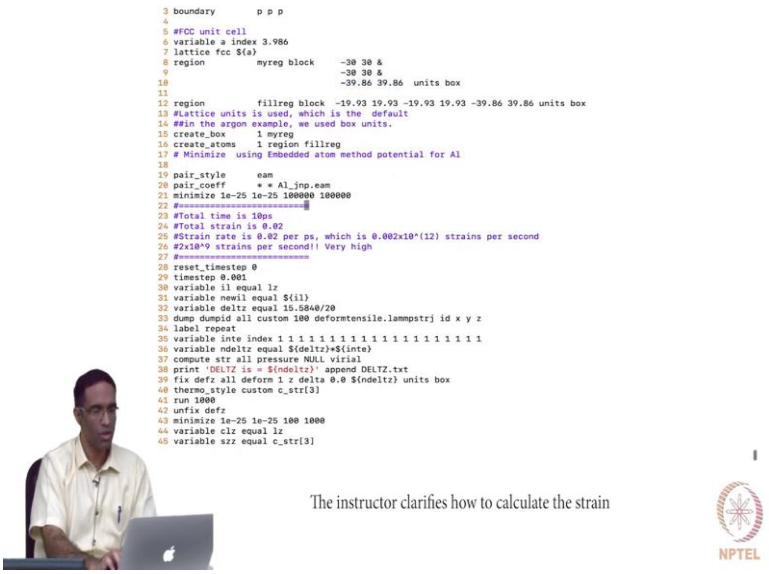

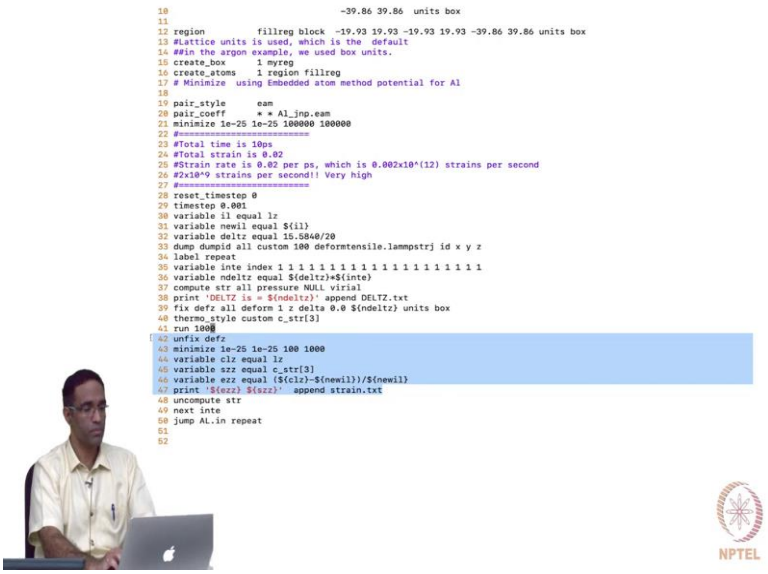

So, in this in the next exercise, in in exercise 15, the strain is calculated in a in a careful way. So, what is happening is/, see you have to think about it a little bit here. So, when it comes to repeat it is going to, this command is going to add the delta z value to the already expanded system, so to the already expanded lz only it is going to add. But the, in the calculation of strain the value that we want to subtract, you know the final length minus the initial length divided by the initial length, this is supposed to be the original 72 point whatever, the, the actual thing that we started off with basically twice 39.86.

So, you have to store that value here. So, il equal lz and new il equal to dollar il. So, when you do this, the new il value does not change. It is fixed to the value that was initialized. So, when you use the dollar new il value, you will be subtracting it from 72 point something, something and here also 72 point something, something and this will be the new length and you will get the corresponding epsilon zz.

This is something that you that I had to work with for some time to actually figure out. So sometimes you have to do some simple tests and make sure that you understand what whatever this gives. Yes?

Student: Sir, we are having such high strain rate?

Professor: Yeah.

Student: Like, minimization will it happen actually like in such a high strain rate...

Professor: No, you are, I am actually applying a strain to deform it to a certain extent. And then minimizing the energy of the system, during the process of tuning usually not much happens because it is quite, because it is, I am not giving any time for the atoms to actually move.

Student: So…

Professor: In the…

Student: Sir, will not the simulation be close to actual when we do not have the minimize, the thing during the preparations, because it seem like it is so high that.

Professor: It is so high. So, in order, if you, I do not I do not understand your question. So, you are telling me, if I did not have the minimization, what would happen?

Student: Like, since the strain rate is so high, minimization will not happen in the actual system.

Professor: Actual means in a real?

Student: Like in the real case, the atom does not have time enough to minimize their value.

Professor: Right, right. So, this is not at that strain rate. This is not at that high strain rate. The total experiment is actually not on an average at that strain rate, because I have a allowed some minimization. If you want the total experiment to be at that strain rate, I should not minimize, I just pull.

Student: But if the simulation itself is having such high strain rate, right?

Professor: This portion, this portion, the small portion, where delta z is added is at a high strain rate, but then I stop it and minimize it. So that basically negates hopefully a little bit of that strain rate, high strain rate effect. The, the average experiment, the computational experiment that we have seen now, the overall experiment is not conducted at a high, at the high strain rate that you would get if you divide the strain amount by the time because you are minimizing in between. However, this is a little bit more realistic of the real system than if you continuously pulled at such high standards because you cannot perform experiments at such high strain rates. So, normally what we do is we actually pull a little bit, minimize it,

pull a little bit minimize it. So, even though the elastic constant determination is the methodology is very clear, the actual simulation can take quite a long time.

Student: Sir, why do…

Student: Sir, where are we defining 2 different region in the script like how outer?

Professor: Good, that is a good question, I think I should have highlighted it. So here, there is a region, I say my region block, and I am giving some arbitrary values minus 30 to 30, minus 30 to 30 in the x and the y directions, and in the z directions it is exactly equal to 20 times the lattice constant. And then I will fill another region and I call it filled region because that is a region I am going to fill, which is smaller than the outer region. But the z direction exactly spans my box. Now, when I say create the box, it creates with my region, when I say create atoms, I fill it inside this. So, it just fills it exactly inside this. So now, this is very nice because when you want to simulate, say a sphere of atoms or put atoms in a cylinder, then you can always define this additional region and fill atoms inside that region.

Student: What would a temperature, the initial temperature of it, does it minimize considering that, here we are not defining anywhere temperature.

Professor: We have not defined, this is just a pure molecular kind of static.

Student: So what, what is the temperature?

Professor: 0 K. Yeah, the atoms are not even vibrating about their mean positions in this case. But if you want more realistic elastic constants to come out of your simulation, you need to include those effects, because the, the expression for elastic constants is not only dependent on positions, but also on the velocities. We have just removed that completely because we just wave our hands and say that for solids it is not that important.

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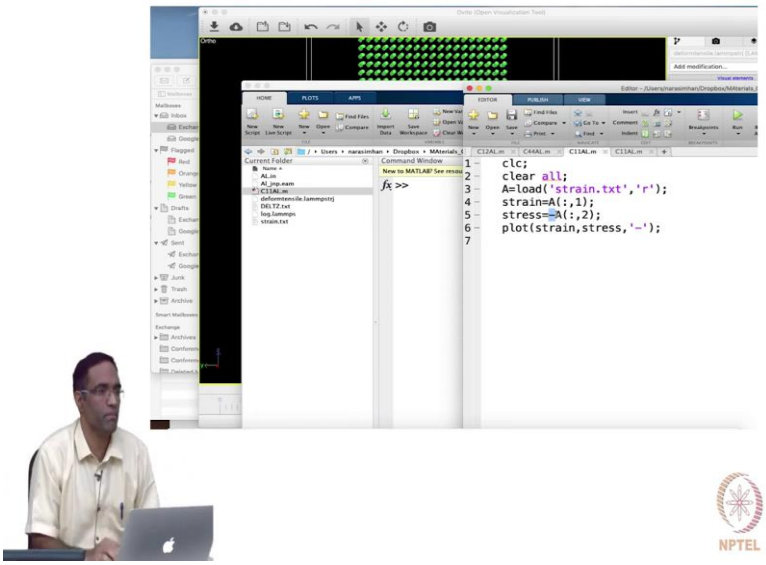

Student: Sir, when you said it is calculating the pressure tensor, pressure is designed to be the (isotropic) isotropic part of the stress tensor.

Professor: No, no, no, it is not that, it is not it is not the hydrostatic part of the, it is not hydrostatic stress. It is, it is stress except there it is having negative, so that is why that is why I added a minus sign in your, in my stress here to make it appear positive because all negative stresses means tensile, positive stresses means, yeah, sorry, yeah negative stresses in in LAMMPS, when it is printing out, it is actually printing out the tensile stresses, this the stress that is acting in the other direction is, is negative.

Student: Pressure it is just calculating sigma.

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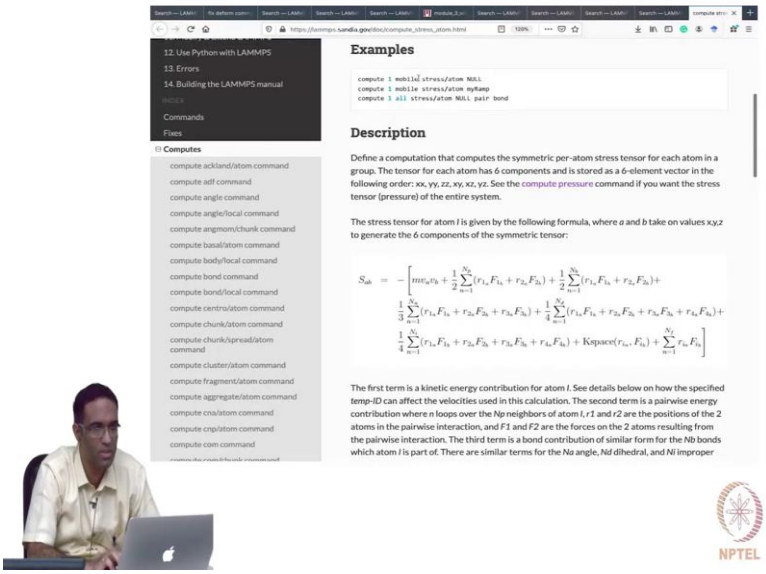

Student: Sir, there is also a compute stress in manual?

Professor: That is compute stress per atom. We do not want that now. Per atom stress, now what that means, I do not know but because you can think about it, what is meant by stress per atom? You still you still can get useful information, for example, if you model a (dislocation), if model a grain boundary, and if you model the stress per atom and average it nicely, you will see the dislocation course alone stress, you must have studied that in some course.

You have stresses emanating from the dislocation core, going reducing as 1 by r square or something like that. So, you can look at all that. So, this is actually the stress that is counted per atom. But that is not what we want, we do not want per atom stress information. We want the stress for the entire simulation boxes and so global quantity, so compute pressure is what is going to do that.