




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

(Refer Slide Time: 0:22)




```

Energy.log           Temperature.tex
Energy.pdf           dump_initial_config.dump
Energy.synctex.gz   forprinting.txt
Energy.tex           input_script.in
Pressure.aux         log.lammps
Pressure.log         logfile.txt
Pressure.pdf         output.txt
Pressure.synctex.gz outputdistgaus.txt
Pressure.tex         thermodynamic_info.txt
Temperature.aux      trj.dump
Temperature.log
Narasimhanhomeair:exercise2 narasimhan$ cd ../
Narasimhanhomeair:Argon narasimhan$ ls
Ar_1000_Kr_0.txt      exercise5
FCC_Argon.in         exercise6
Icon?                 exercise7
Important_Argon_Paper_2017.pdf exercise8
dump.eqm1            exercise9
dump.eqm2            exerciserdf
dump.eqm3            exerciserdfgas
dump.min             inputl_argon.in
exercisel1           log.lammps
exercisel10          log_n_ar_1000.txt
exercisel2           logfile.txt
exercisel3           output.out
exercisel4
Narasimhanhomeair:Argon narasimhan$ cd exercisel1
Narasimhanhomeair:exercisel1 narasimhan$ ls
dump.min             input_script.in log.lammps logfile.txt output.txt
Narasimhanhomeair:exercisel1 narasimhan$ ls
ump.min              input_script.in log.lammps logfile.txt output.txt
Narasimhanhomeair:exercisel1 narasimhan$ vim input_script.in
Narasimhanhomeair:exercisel1 narasimhan$ █
  
```

```

58 #<dump ID group style N filename args. See web page for details. ix iy and iz give the
    details of the image that the atom is presently located>
59 #=====
60 run 1
61 minimize 1e-7 1e-9 10000 10000 #<Minimize the energy using a conjugate gradient step.
62 print "Finished Minimizing"
63 #minimize etol ftol maxiter for minimizer maxiter for force_energy valuation
64 #dump dump_1 all custom 1 dump.min id type x y z ix iy iz vx vy vz #<Dump all the atom
    s to the file dump.min>
65 #=====
66 #log file_two.txt
67 # Open another logfile for printing thermodynamic information, from this point onwards
.
68 thermo_style custom step time temp pe etotal press vol
69 #What to print in the logfile.txt?
70 #=====
71 velocity all create 300 102939 dist gaussian mom yes rot yes
72 # Set the velocities of all the atoms so that the temperature of the system
73 # is 300K. Make the distribution Gaussian.
74 thermo 1 #How frequently to print the thermodynamic information#
75 variable t equal time
76 run ${stp} # run with active settings as many runs as required.
77 #run ${stp} every 10 *print '-----Time is $t' " # run as man
    y steps as defined using the variable stp
78 #and then every 10 steps print the time.
79 #If the name of the variable is a single character, you need not use the
80 #flower brackers "{}".
81 undump dump_1 # Stop dumping information to the dump file.
82 print "Printed in the new log file"
83 print "None of the atoms vibrate"
84 print "Need to have a fix"
85 #print something.
  
```




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.


(Refer Slide Time: 1:25)

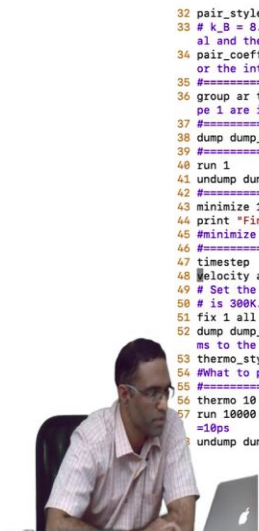


```
dump.min          input1_argon.in
exercise1         log.lammps
exercise10        log.n_ar_1000.txt
exercise2         logfile.txt
exercise3         output.out
exercise4
Narasimhanhomeair:Argon narasimhan$ cd exercise1
Narasimhanhomeair:exercise1 narasimhan$ ls
dump.min          input_script.in log.lammps      logfile.txt      output.txt
Narasimhanhomeair:exercise1 narasimhan$ ls
dump.min          input_script.in log.lammps      logfile.txt      output.txt
Narasimhanhomeair:exercise1 narasimhan$ vim input_script.in
Narasimhanhomeair:exercise1 narasimhan$ ls
dump.min          input_script.in log.lammps      logfile.txt      output.txt
Narasimhanhomeair:exercise1 narasimhan$ cd ../
Narasimhanhomeair:Argon narasimhan$ ls
Ar_1000_Kr_0.txt  exercise5
FCC_Argon.in     exercise6
Icon?            exercise7
Important_Argon_Paper_2017.pdf exercise8
dump.eqm1        exercise9
dump.eqm2        exerciserdf
dump.eqm3        exerciserdfgas
dump.min         input1_argon.in
exercise1        log.lammps
exercise10       log.n_ar_1000.txt
exercise2        logfile.txt
exercise3        output.out
exercise4
Narasimhanhomeair:Argon narasimhan$ pwd
/Users/narasimhan/OneDrive - IIT-Madras(IC&SR)/Research_folder/MATerials_Course/Molecular_Dynamic/Argon
Narasimhanhomeair:Argon narasimhan$ cd
```



```
1 ## Is a comment line
2 # (1) System creation of FCC of ARGON lattice
3 # (2) Specification of potential type and cut off
4 # (3) CG energy minimization
5 # (4) Printing of coordinate information
6 # (5) Printing of thermodynamic information
7 # (6) Visualization of coordinates and some options in Ovito
8 # (7) Any line beginning with a # is a comment
9 # (8) Any line ending with '&' means the command continues in the next line
10 ##
11 #=====
12 #
13 units          metal #<What are the units you will use to specify various things in t
he input file?
14 #Look at the link <https://lammps.sandia.gov/doc/units.html>
15 boundary       p p p #<Specify periodic boundary condition are needed in all three fa
ces of the simulation box>
16 atom_style     atomic #<What style of atoms is to be used in the simulation>
17 log            logfile.txt #<write the log file to this text file.All thermodynamic i
nformation applicable to the entire system>
18 #=====
19 region forbox block 0 45.8 0 45.8 0 45.8 units box
20 #<Refers to an abstract geometric region of space. units box refers to the fact that t
he size of the box is specified in the units as given in the units command. The name "
forbox" refers to the region ID so that you can refer to it somewhere else in this inp
ut script.>
21 create_box 1 forbox #<Create the box>
22 #=====
23 #<Creates the lattice> <4.85 is the argument for the scale keyword, while the other a1
, a2 a3 are the three lattice vectors: This is followed by the basis commands giving th
e location of atoms in one unit cell.>
24 lattice custom 4.85 a1 1.0 0.0 0.0 a2 0.0 1.0 0.0 a3 0.0 0.0 1.0 &
"input_script.in" [dos] 61L, 3986C
```


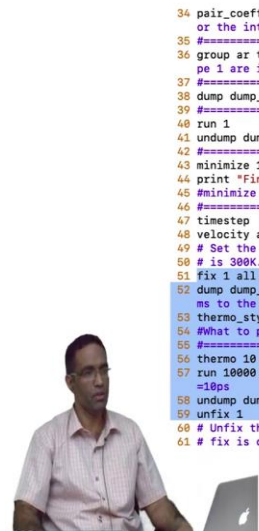




```

32 pair_style      lj/cut 10
33 # k_B = 8.6173308e-5 eV/K #<How are atoms interacting. Provide the name of the potenti
al and the corresponding cut-off distance>
34 pair_coeff      1 1      0.01006418      3.3952 #<The coefficient of the lj potential f
or the interactions of atom type 1 with 1>
35 #=====
36 group ar type 1 #<Group all the argon types (argon type is of type 1). All atoms of ty
pe 1 are in group with the name 'ar'
37 #=====
38 dump dump_1 all custom 1 dump_initial_config.dump id type x y z ix iy iz vx vy vz
39 #=====
40 run 1
41 undump dump_1 # Stop dumping to this file
42 #=====
43 minimize 1e-7 1e-9 10000 10000 #<Minimize the energy using a conjugate gradient step.
44 print "Finished Minimizing"
45 #minimize etol ftol maxiter for minimizer maxiter for force_energy valuation
46 #=====
47 timestep 0.001
48 velocity all create 300 102930 dist gaussian mom yes rot yes
49 # Set the velocities of all the atoms so that the temperature of the system
50 # is 300K. Make the distribution Gaussian.
51 fix 1 all nve
52 dump dump_1 all custom 100 trj.dump id type x y z ix iy iz vx vy vz #<Dump all the ato
ms to the file dump.min>
53 thermo_style custom step time temp pe ke etotal press vol
54 #What to print in the logfile.txt?
55 #=====
56 thermo 10 #How frequently to print the thermodynamic information#
57 run 10000 # run with active settings as many runs as required. timestep*No. of. steps
=10ps
58 undump dump_1 # Stop dumping information to the dump file.


```

```

34 pair_coeff      1 1      0.01006418      3.3952 #<The coefficient of the lj potential f
or the interactions of atom type 1 with 1>
35 #=====
36 group ar type 1 #<Group all the argon types (argon type is of type 1). All atoms of ty
pe 1 are in group with the name 'ar'
37 #=====
38 dump dump_1 all custom 1 dump_initial_config.dump id type x y z ix iy iz vx vy vz
39 #=====
40 run 1
41 undump dump_1 # Stop dumping to this file
42 #=====
43 minimize 1e-7 1e-9 10000 10000 #<Minimize the energy using a conjugate gradient step.
44 print "Finished Minimizing"
45 #minimize etol ftol maxiter for minimizer maxiter for force_energy valuation
46 #=====
47 timestep 0.001
48 velocity all create 300 102939 dist gaussian mom yes rot yes
49 # Set the velocities of all the atoms so that the temperature of the system
50 # is 300K. Make the distribution Gaussian.
51 fix 1 all nve
52 dump dump_1 all custom 100 trj.dump id type x y z ix iy iz vx vy vz #<Dump all the ato
ms to the file dump.min>
53 thermo_style custom step time temp pe ke etotal press vol
54 #What to print in the logfile.txt?
55 #=====
56 thermo 10 #How frequently to print the thermodynamic information#
57 run 10000 # run with active settings as many runs as required. timestep*No. of. steps
=10ps
58 undump dump_1 # Stop dumping information to the dump file.
59 unfix 1
60 # Unfix the NVE. Additional lines if any will assume that this
61 # fix is off

```



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.

(Refer Slide Time: 5:41)

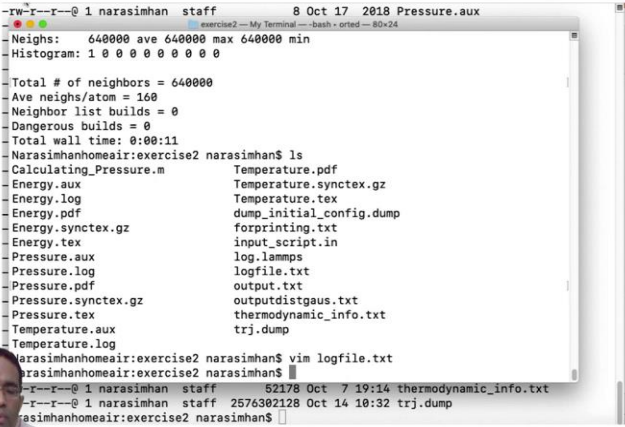
```
227 | 998      0.989   152.34233  274.13844  78.747477  352.87792  78514.026
    | 96871.912
228 | 1000     0.999   152.0536   274.27895  78.598226  352.87718  78523.551
    | 96871.912
229 | 1002     1.001   152.00115  274.30601  78.571114  352.87712  78525.206
    | 96871.912
230 | Loop time of 11.3296 on 1 procs for 1000 steps with 4000 atoms
231 |
232 | Performance: 7.626 ns/day, 3.147 hours/ns, 88.264 timesteps/s
233 | 96.6% CPU use with 1 MPI tasks x no OpenMP threads
234 |
235 | MPI task timing breakdown:
236 | Section | min time | avg time | max time | %varavg | %total
237 |-----|-----|-----|-----|-----|-----
238 | Pair    | 11.002   | 11.002   | 11.002   | 0.0     | 97.11
239 | Neigh   | 0        | 0        | 0        | 0.0     | 0.00
240 | Comm   | 0.091293 | 0.091293 | 0.091293 | 0.0     | 0.81
241 | Output | 0.12635  | 0.12635  | 0.12635  | 0.0     | 1.12
242 | Modify | 0.070998 | 0.070998 | 0.070998 | 0.0     | 0.63
243 | Other  | 0.03917  | 0.03917  | 0.03917  | 0.0     | 0.35
244 |
245 | Nlocal: 4000 ave 4000 max 4000 min
246 | Histogram: 1 0 0 0 0 0 0 0
247 | Nghost: 10895 ave 10895 max 10895 min
248 | Histogram: 1 0 0 0 0 0 0 0
249 | Neighs: 640000 ave 640000 max 640000 min
250 | Histogram: 1 0 0 0 0 0 0 0
251 |
252 | Total # of neighbors = 640000
253 | Ave neighs/atom = 160
254 | Neighbor list builds = 0
255 | Dangerous builds = 0
```





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.

(Refer Slide Time: 7:12)

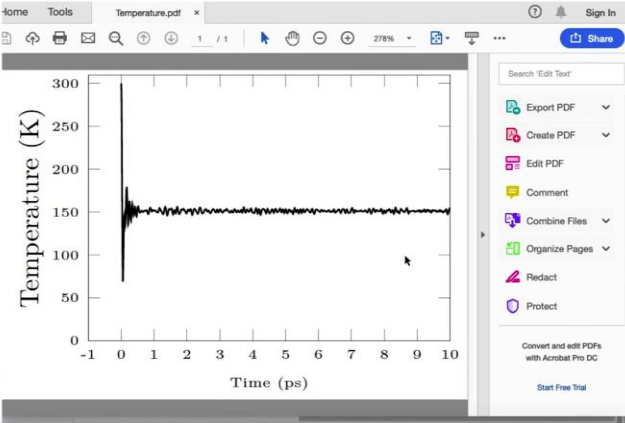


```
-rw-r--r--@ 1 narasimhan staff      8 Oct 17 2018 Pressure.aux
exercise2 - My Terminal - bash - orted - 80x24
Neighs: 640000 ave 640000 max 640000 min
Histogram: 1 0 0 0 0 0 0 0 0
Total # of neighbors = 640000
Ave neighs/atom = 160
Neighbor list builds = 0
Dangerous builds = 0
Total wall time: 0:00:11
Narasimhanhomeair:exercise2 narasimhan$ ls
Calculating_Pressure.m      Temperature.pdf
Energy.aux                 Temperature.synctex.gz
Energy.log                 Temperature.tex
Energy.pdf                 dump_initial_config.dump
Energy.synctex.gz          forprinting.txt
Energy.tex                 input_script.in
Pressure.aux               log_lammps
Pressure.log               logfile.txt
Pressure.pdf               output.txt
Pressure.synctex.gz        outputdistgaus.txt
Pressure.tex               thermodynamic_info.txt
Temperature.aux            trj.dump
Temperature.log
Narasimhanhomeair:exercise2 narasimhan$ vim logfile.txt
Narasimhanhomeair:exercise2 narasimhan$
-rw-r--r--@ 1 narasimhan staff      52178 Oct 7 19:14 thermodynamic_info.txt
-rw-r--r--@ 1 narasimhan staff 2576302128 Oct 14 10:32 trj.dump
Narasimhanhomeair:exercise2 narasimhan$
```





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.

(Refer Slide Time: 7:58)



The figure shows a plot of Temperature (K) versus Time (ps). The y-axis ranges from 0 to 300 K, and the x-axis ranges from -1 to 10 ps. The plot shows a sharp initial spike in temperature reaching approximately 300 K at time 0, followed by a rapid decay and stabilization around 150 K. The temperature remains constant with minor fluctuations between 140 K and 160 K for the remainder of the 10 ps duration.



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?

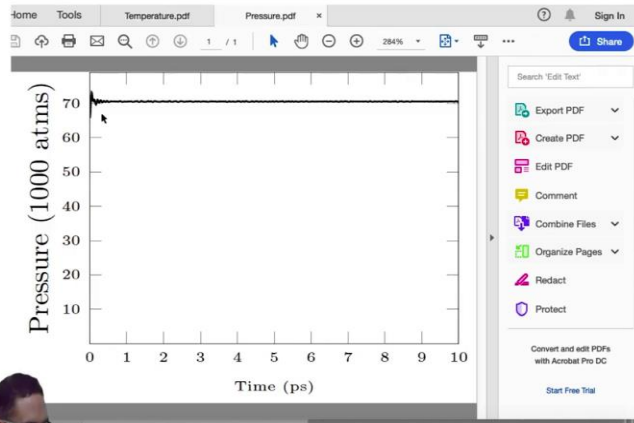
Student: Energy conservation between kinetic and potential energy

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.

(Refer Slide Time: 11:31)



```



121 thermo_style custom step time temp pe ke etotal press vol
122 #What to print in the logfile.txt?
123 #=====
124 thermo 10 #How frequently to print the thermodynamic information#
125 run 1000 # run with active settings as many runs as required. timestep#No. of. steps =
126 Per MPI rank memory allocation (min/avg/max) = 5.878 | 5.878 | 5.878 Mbytes
127 Step Time Temp PotEng KinEng TotEng Press Volume
128 2 0.001 300 197.81322 155.0734 352.88661 65748.927
129 96071.912
130 10 0.009 286.60924 204.73625 148.15156 352.88781 66184.834
131 96071.912
132 20 0.019 236.73941 230.51955 122.37328 352.89283 67804.935
133 96071.912
134 30 0.029 166.36613 266.89997 85.996534 352.89651 70882.173
135 96071.912
136 40 0.039 102.22635 300.04704 52.841959 352.889 72147.541
137 96071.912
138 50 0.049 68.962321 317.23986 35.647404 352.88726 73211.137
139 96071.912
140 60 0.059 72.995751 315.15189 37.73233 352.88422 73070.594
141 96071.912
142 70 0.069 99.984638 301.19326 51.683191 352.87645 72188.547
143 96071.912
144 80 0.079 128.78259 286.30759 66.569181 352.87678 71249.042
145 96071.912
146 90 0.089 145.32478 277.75438 75.120022 352.8744 70710.345
147 96071.912
148 100 0.099 147.01467 276.88068 75.993547 352.87423 70659.718
149 96071.912
150 110 0.109 140.1193 280.44413 72.429255 352.87339 70893.353
151 96071.912

```



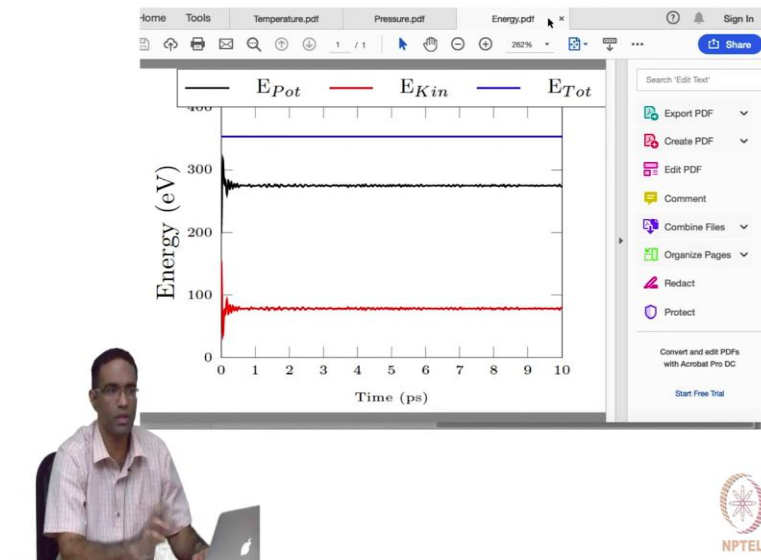
215	870	0.869	154.19407	273.17285	79.704662	352.87751	70452.503
	96071.912						
216	880	0.879	155.14823	272.67979	80.197878	352.87767	70421.419
	96071.912						
217	890	0.889	155.18314	272.66181	80.21592	352.87773	70420.385
	96071.912						
218	900	0.899	154.33001	273.10463	79.774927	352.87955	70448.305
	96071.912						
219	910	0.909	152.93013	273.82276	79.051317	352.87892	70493.688
	96071.912						
220	920	0.919	151.54088	274.54782	78.333197	352.88101	70538.459
	96071.912						
221	930	0.929	150.73302	274.96204	77.915604	352.87765	70564.006
	96071.912						
222	940	0.939	150.7552	274.94878	77.927068	352.87584	70562.829
	96071.912						
223	950	0.949	151.37404	274.63081	78.246953	352.87777	70542.779
	96071.912						
224	960	0.959	152.08673	274.26309	78.615351	352.87844	70520.041
	96071.912						
225	970	0.969	152.50128	274.0507	78.829637	352.88034	70507.345
	96071.912						
226	980	0.979	152.54544	274.02756	78.852462	352.88002	70506.779
	96071.912						
227	990	0.989	152.34233	274.13044	78.747477	352.87792	70514.026
	96071.912						
228	1000	0.999	152.0536	274.27895	78.598226	352.87718	70523.551
	96071.912						
229	1002	1.001	152.00115	274.30601	78.571114	352.87712	70525.206
	96071.912						

Loop time of 11.3296 on 1 procs for 1000 steps with 4000 atoms

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.

(Refer Slide Time: 12:26)

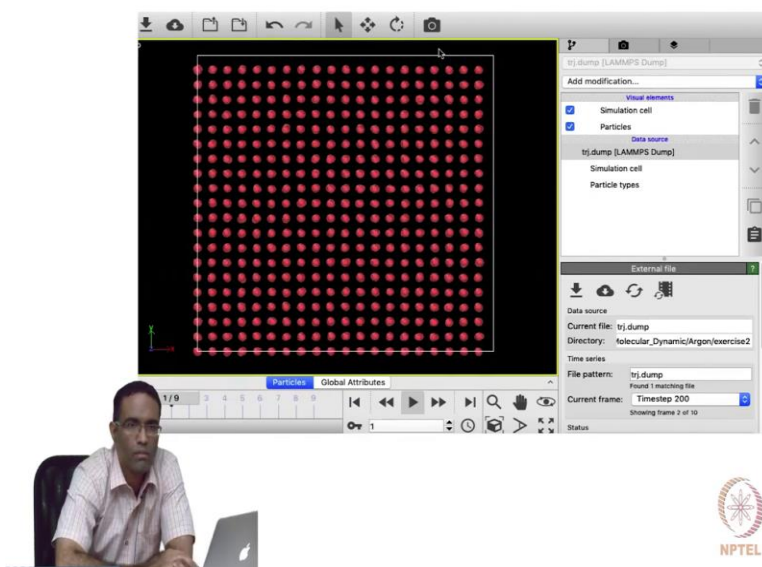


If you look at the energy, so this is the energy distribution. So you started off with this is the potential energy part, this is the kinetic energy part. This is what you gave initially and then it

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?

(Refer Slide Time: 13:42)



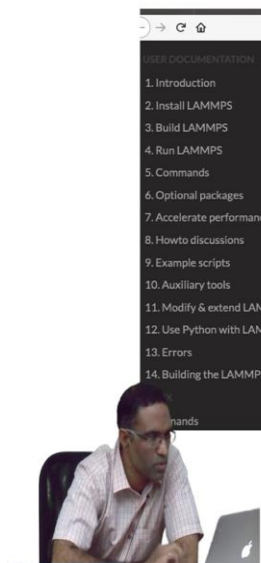

So now let us take a look at our trajectory and see if, so you can see some moment in contrast to what you saw yesterday where the atoms they were not moving at all. So this is essentially because now the atoms are being integrated and you are getting new positions and velocities for all these atoms 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?

(Refer Slide Time: 14:44)



```
-rw-r--r--@ 1 narasimhan staff 8 Oct 17 2018 Pressure.aux
exercise2 - My Terminal - vi input_script.in - 80x24
42 #=====
43 minimize 1e-7 1e-9 10000 10000 #<Minimize the energy using a conjugate gradient step.
44 print "Finished Minimizing"
45 #minimize etol ftol maxiter for minimizer maxiter for force_energy valuation
46 #=====
47 timestep 0.001
48 velocity all create 300 102939 dist gaussian mom yes rot yes
49 # Set the velocities of all the atoms so that the temperature of the system
50 # is 300K. Make the distribution Gaussian.
51 fix 1 all nve
52 dump dump_1 all custom 100 trj.dump id type x y z ix iy iz vx vy vz #<Dump all the atoms to the file dump.min>
53 thermo_style custom step time temp pe ke etotal press vol
54 #What to print in the logfile.txt?
55 #=====
56 thermo 10 #How frequently to print the thermodynamic information#
57 run 1000 # run with active settings as many runs as required. timestep*No. of steps =10ps
58 undump dump_1 # Stop dumping information to the dump file.
59 unfix
60 # Unfix the NVE. Additional lines if any will assume that this
61 # fix is off.

-rw-r--r--@ 1 narasimhan staff 52178 Oct 7 19:14 thermodynamic_info.txt
-rw-r--r--@ 1 narasimhan staff 2576302128 Oct 14 10:32 trj.dump
Narasimhan@homeair:exercise2 narasimhan$
```



https://lammps.sandia.gov/doc/fix_nve.html

Previous

fix nve command

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



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

INDEX
Commands

Fixes
adapt command
adapt/feq command

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
```



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 bocc command
fix bond/break command
fix bond/create command
fix bond/swap command
fix bond/react command
fix box/relax command


fix nvt 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
tcchain 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



fix edpd/source command
fix tdpd/source command
fix dt/reset command
fix efield command
fix ehex command
fix electron/stopping command
fix enforce2d command
fix enforce2d/kk command
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 fff 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
```


fix nph command

Description

These commands perform time integration on Nose-Hoover style non-Hi are designed to generate positions and velocities sampled from the canonical [isenthalpic \(nph\) ensemble](#). This updates the position and velocity for at

The thermostating and barostatting is achieved by adding some dynamic particle velocities (thermostating) and simulation domain dimensions (b thermostating and barostatting, these fixes can also create a chain of the thermostat, and another chain of thermostats coupled to the barostat via the overall box volume, or to individual dimensions, including the xy, xz or pressure of the barostat can be specified as either a scalar pressure (isob symmetric stress tensor (constant stress ensemble). When used correctly 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 I



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.

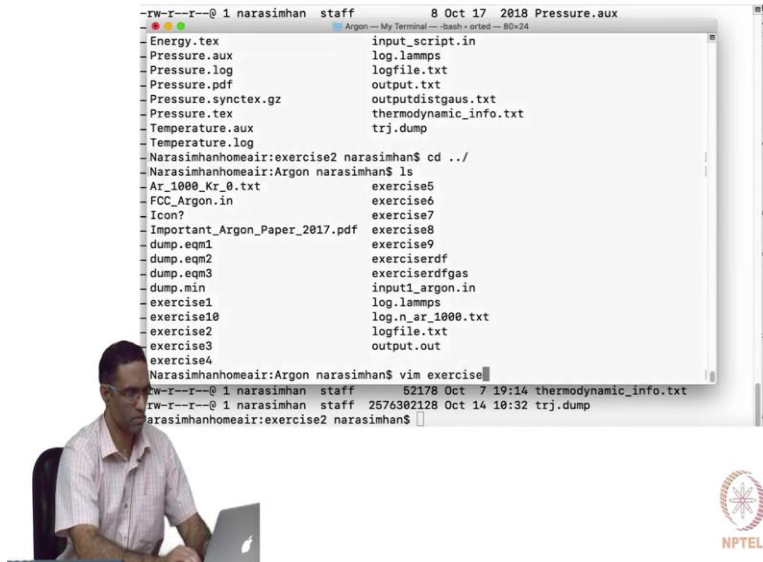
There is the ID for the fix, the corresponding group ID and followed by nve is what you need in order to run this. But this is just going to perform a simple integration, there is nothing more to it. But if you want to now bring the system to a specific temperature, then you need to couple the existing 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.

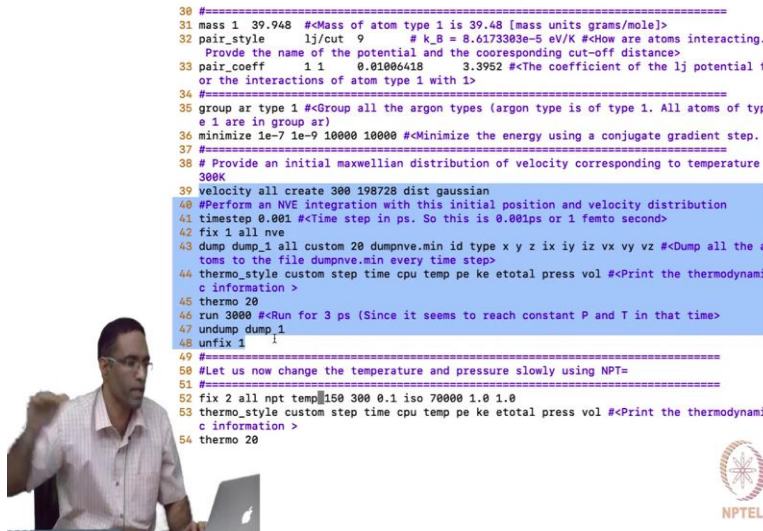
Student: Sir h stands for?

Professor: Enthalpy, isenthalpic.

(Refer Slide Time: 17:22)

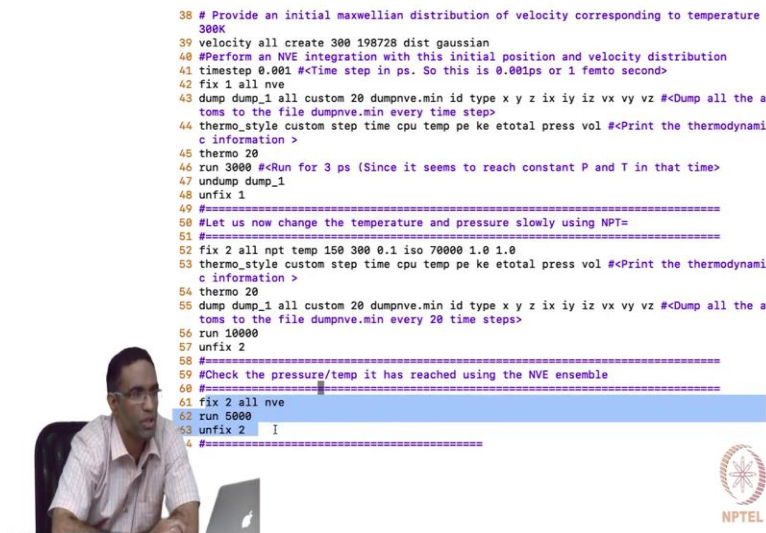


```
-rw-r--r--@ 1 narasimhan staff      8 Oct 17  2018 Pressure.aux
Energy.tex          input_script.in
Pressure.aux        log.lammps
Pressure.log        logfile.txt
Pressure.pdf        output.txt
Pressure.synctex.gz outputdistgaus.txt
Pressure.tex        thermodynamic_info.txt
Temperature.aux     trj.dump
Temperature.log
Narasimhanhomeair:exercise2 narasimhan$ cd ../
Narasimhanhomeair:Argon narasimhan$ ls
Ar_1000_Kr_0.txt    exercise5
FCC_Argon.in        exercise6
Icon?               exercise7
Important_Argon_Paper_2017.pdf exercise8
-dump.eqm1          exercise9
-dump.eqm2          exerciserdf
-dump.eqm3          exerciserdfgas
-dump.min           input1_argon.in
-exercise1          log.lammps
-exercise10         log.n_ar_1000.txt
-exercise2          logfile.txt
-exercise3          output.out
-exercise4
Narasimhanhomeair:Argon narasimhan$ vim exercise
-rw-r--r--@ 1 narasimhan staff      52178 Oct  7 19:14 thermodynamic_info.txt
-rw-r--r--@ 1 narasimhan staff    2576302128 Oct 14 10:32 trj.dump
Narasimhanhomeair:exercise2 narasimhan$
```



```
30 #=====
31 mass 1 39.948 #<Mass of atom type 1 is 39.48 [mass units grams/mole]>
32 pair_style lj/cut 9 # k_B = 8.6173303e-5 eV/K #<How are atoms interacting.
Provide the name of the potential and the corresponding cut-off distance>
33 pair_coeff 1 1 0.81006418 3.3952 #<The coefficient of the lj potential f
or the interactions of atom type 1 with 1>
34 #=====
35 group ar type 1 #<Group all the argon types (argon type is of type 1. All atoms of typ
e 1 are in group ar)
36 minimize 1e-7 1e-9 10000 10000 #<Minimize the energy using a conjugate gradient step.
37 #=====
38 # Provide an initial maxwellian distribution of velocity corresponding to temperature
300K
39 velocity all create 300 198728 dist gaussian
40 #Perform an NVE integration with this initial position and velocity distribution
41 timestep 0.001 #<Time step in ps. So this is 0.001ps or 1 femto second>
42 fix 1 all nve
43 dump dump_1 all custom 20 dumpnve.min id type x y z ix iy iz vx vy vz #<Dump all the a
toms to the file dumpnve.min every time step>
44 thermo_style custom step time cpu temp pe ke etotal press vol #<Print the thermodynami
c information >
45 thermo 20
46 run 3000 #<Run for 3 ps (Since it seems to reach constant P and T in that time)
47 undump dump_1
48 unfix 1
49 #=====
50 #Let us now change the temperature and pressure slowly using NPT=
51 #=====
52 fix 2 all npt temp=150 300 0.1 iso 70000 1.0 1.0
53 thermo_style custom step time cpu temp pe ke etotal press vol #<Print the thermodynami
c information >
54 thermo 20
```



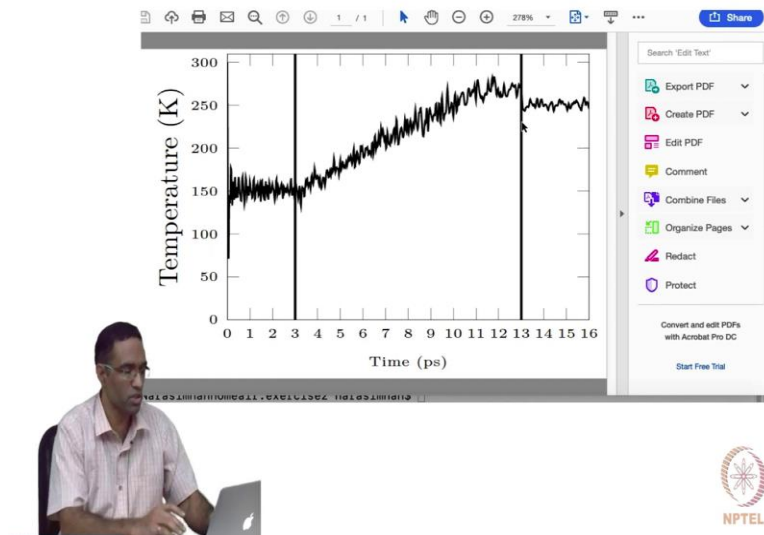


So if you have, so let me open that, let me see if I have a. So in this case, what I do, almost everything is the same. I provide initial velocity. And I print out some information here. Now I want to change the temperature slowly and the pressure slowly. So fix 2 all. I use npt, I changed the temperature 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.

(Refer Slide Time: 19:40)



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.

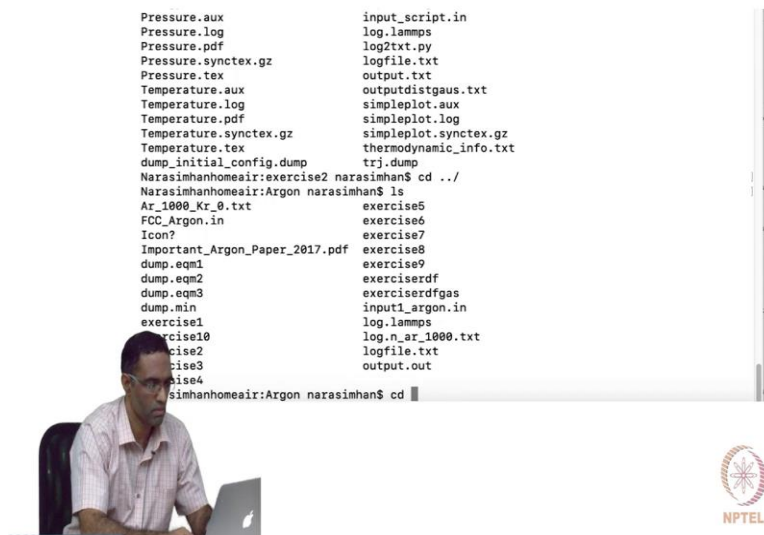
Student: Sir, so if we increase the number of iterations in the simulation the command we say the pressure is 1 bar and the temperature is more than 300, make the iterations, more iterations.

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.

(Refer Slide Time: 24:36)



```

41 timestep 0.001 #<Time step in ps. So this is 0.001ps or 1 femto second>
42 fix 1 all nve
43 dump dump_1 all custom 20 dumpnve.min id type x y z ix iy iz vx vy vz #<Dump all the
atoms to the file dumpnve.min every time step>
44 thermo_style custom step time cpu temp pe ke etotal press vol #<Print the thermodyna
mic information >
45 thermo 20
46 run 3000 #<Run for 3 ps (Since it seems to reach constant P and T in that time>
47 undump dump_1
48 unfix 1
49 #=====
50 #Let us now change the temperature and pressure slowly using NPT=
51 #=====
52 fix 2 all npt temp 150 300 0.1 iso 70000 1.0 1.0
53 thermo_style custom step time cpu temp pe ke etotal press vol #<Print the thermodyna
mic information >
54 thermo 20
55 dump dump_1 all custom 20 dumpnve.min id type x y z ix iy iz vx vy vz #<Dump all the
atoms to the file dumpnve.min every 20 time steps>
56 run 10000
57 unfix 2
58 #=====
59 #Check the pressure/temp it has reached using the NVE ensemble
60 #=====
fix 2 all nve
run 5000

```



LAMMPS

Search box

- 1. Introduction
- 2. Install LAMMPS
- 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

time units (e.g. tau or femsec or psec - see the units command). The atoms in the fix group are the only ones whose velocity/position update portion of the integration.

Note

A Nose-Hoover thermostat will not work well for arbitrary values of T_{damp} . If T_{damp} is too small, the temperature will take a very long time to equilibrate. A good choice for many models is a T_{damp} of around 100 timesteps. Note units settings. A simple way to ensure this, is via using an *immediate* variable expression accessing the thermo proc

```
fix 1 all nvt temp 300.0 300.0 5[100.0*dt]
```

The barostat parameters for fix styles npt and nph is specified using one or more of the iso, aniso, tri,x,y,z,xy,xz,yz, to specify all 6 components of an external stress tensor, and to couple various of these components together so that during a constant-pressure simulation.

Other barostat-related keywords are pchain, mtz, ploop, nreset, drag, and dilate, which are discussed below.

Orthogonal simulation boxes have 3 adjustable dimensions (x,y,z). Triclinic (non-orthogonal) simulation boxes have read data, and read_restart commands specify whether the simulation box is orthogonal or non-orthogonal (triclinic)

The target pressures for each of the 6 components of the stress tensor can be specified independently via the x,y,z simulation box dimensions. For each component, the external pressure or tensor component at each timestep is a r target pressure is specified for a component, then the corresponding box dimension will change during a simulator will change. If the xy keyword is used, the xy tilt factor will change. A box dimension will not change if that compone change that dimension via the fix deform command.



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.

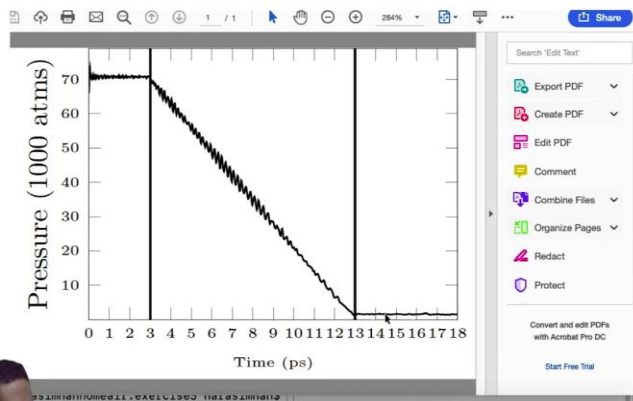
Too high value essentially means that you are forcing the pressure to come to the value that you require very quickly and you will see huge fluctuations in the pressure. And if you give too lower value then it will take a very very long time for it to actually reach the pressure that you are requesting. 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.

(Refer Slide Time: 27:20)

```
43 dump dump_1 all custom 20 dumpvne.min id type x y z ix iy iz vx vy vz #<Dump all the
   atoms to the file dumpvne.min every time step>
44 thermo_style custom step time cpu temp pe ke etotal press vol #<Print the thermodyna
   mic information >
45 thermo 20
46 run 3000 #<Run for 3 ps (Since it seems to reach constant P and T in that time>
47 undump dump_1
48 unfix 1
49 #=====
50 #Let us now change the temperature and pressure slowly using NPT=
51 #=====
52 fix 2 all npt temp 150 300 0.1 iso 70000 1.0 1.0
53 thermo_style custom step time cpu temp pe ke etotal press vol #<Print the thermodyna
   mic information >
54 thermo 20
55 dump dump_1 all custom 20 dumpvne.min id type x y z ix iy iz vx vy vz #<Dump all the
   atoms to the file dumpvne.min every 20 time steps>
56 run 10000
57 unfix 2
58 #=====
59 #Check the pressure/temp it has reached using the NVE ensemble
60 #=====
61 fix 2 all nve
62 run 5000
63 unfix 2
64 #=====
```





```

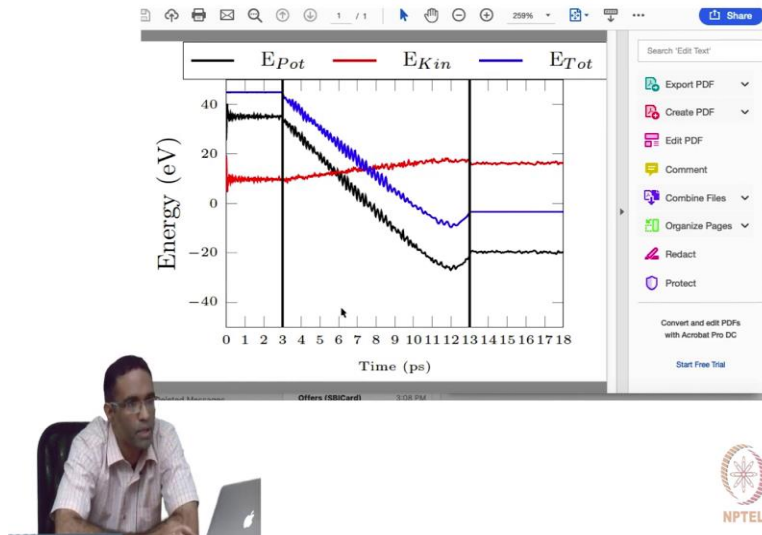
823 unfix 2
824 #=====
825 #Check the pressure/temp it has reached using the NV ensemble
826 #=====
827 fix 2 all nve
828 run 5000
829 Per MPI rank memory allocation (min/avg/max) = 4.487 | 4.487 | 4.487 Mbytes
830 Step Time CPU Temp PotEng KinEng TotEng Press Volume
831 13001 13 0 273.69156 -21.038903 17.653328 -3.3855
832 751 1077.7582 28100.888
13020 13.019 0.0061671734 265.55862 -20.513269 17.128747 -3.3845
833 223 1231.2832 28100.888
13040 13.039 0.012748003 255.6659 -19.872377 16.498658 -3.3817
834 193 1411.3555 28100.888
13060 13.059 0.019309998 248.01961 -19.377428 15.997466 -3.3799
835 619 1556.0699 28100.888
13080 13.079 0.025935173 245.13877 -19.192452 15.81165 -3.380
836 802 1628.2798 28100.888
13100 13.099 0.032528162 245.10077 -19.191772 15.809199 -3.3825
837 735 1654.4706 28100.888
13120 13.119 0.039587021 244.80806 -19.171163 15.790319 -3.3808
838 442 1678.9097 28100.888
13140 13.139 0.045825005 243.76073 -19.103012 15.722765 -3.3802
839 476 1708.8135 28100.888
13160 13.159 0.052061081 243.52882 -19.088393 15.707806 -3.3805
862 1722.7179 28100.888

```



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.

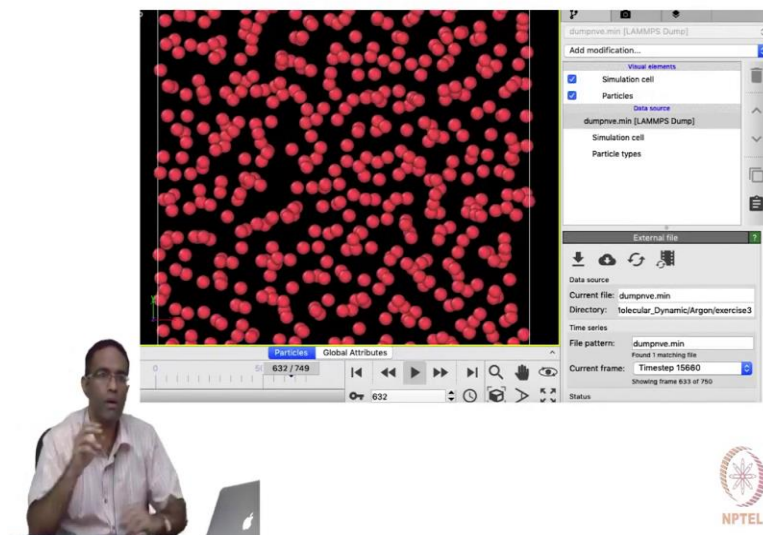
(Refer Slide Time: 28:27)



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.

(Refer Slide Time: 29:25)



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 when you do nvt alone, the volume 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 they 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.