Foundations of Computational Materials Modelling
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Input script for LAMMPS 2

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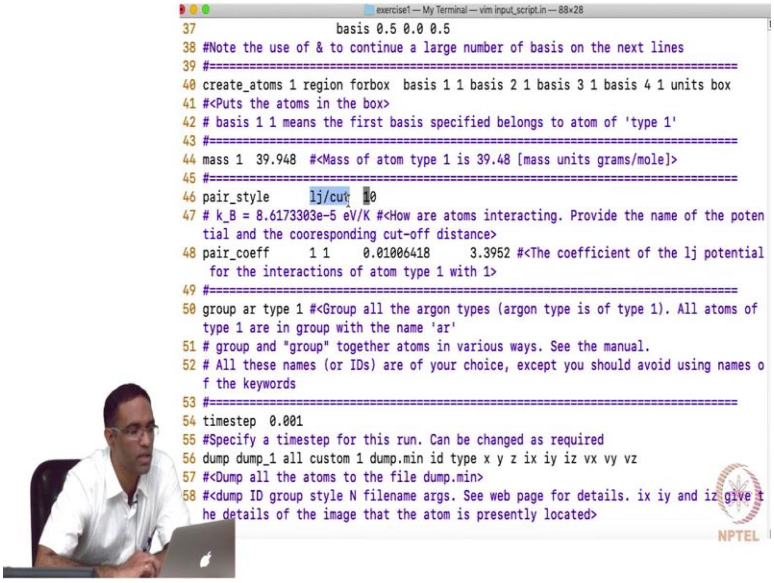

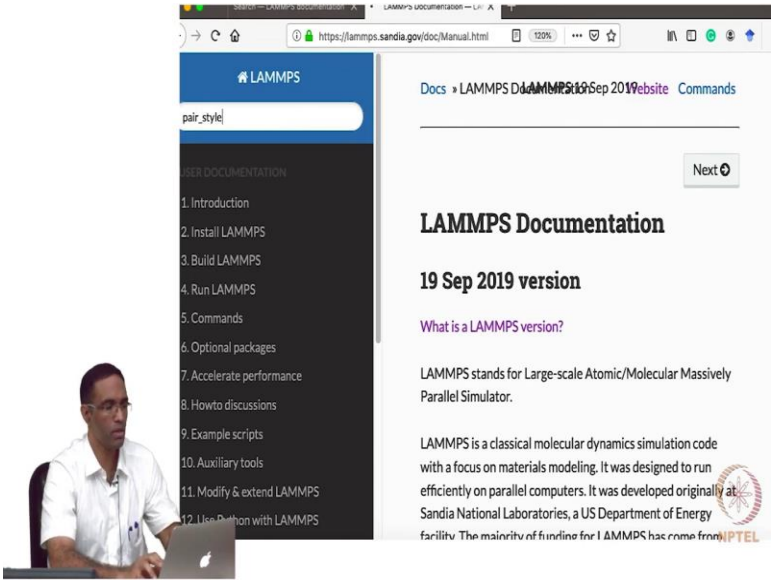

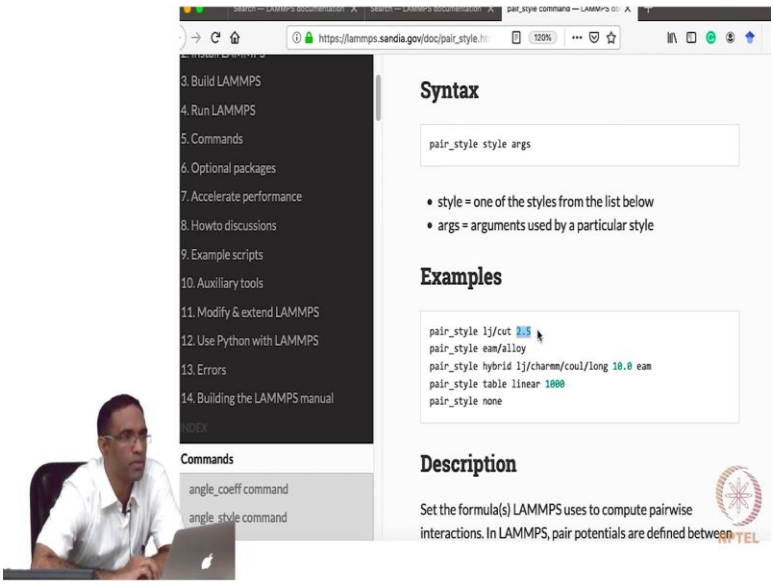

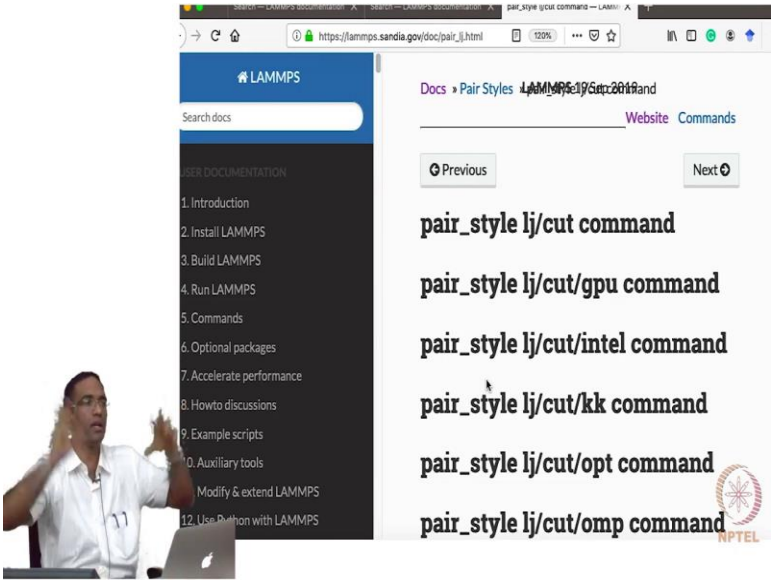

I think we stopped at this particular command right here, how we actually put the atoms of the system into a box, of a given region. This is where we stop the remember right, after that what we do is we essentially I have to assign one of the most important things that you have to give properties that you have to give your atoms is the mass of the atom. So, you say mass that atom type. So, there are only there is only one type of atom in the system which is basically the argon atom. So, you say mass 1 and the corresponding mass of the system in mass units for this units that you have specified, which is going to be in grams per mole, we can find all this information in standard places.

Once we have specified the mass, we specify the inter atomic potential, the manner in which the various atoms in the system had to interact. So, like I mentioned, we are talking about a noble, we are talking about argon, noble gas, but of course we are going to not look at its behavior at higher temperatures now, we have constructed argon as FCCs, FCC using FCC lattice treating it as if it were a solid maybe at extremely low temperatures it behaves as a solid. But that is just used for explaining this input file. Pair style is given as pair style is basically the key word and what is the type of the pair style interaction.

So, in this case I have used LJ slash cut. So, LJ is obviously for Lennard-jones, but this is actually an important keyword and therefore we can actually take a look at the manual for this particular command. So, pair style, style, so what is what are the various styles and they can be a huge list here. And the various arguments that are required for a particular style. So, for example if it is LJ slash cut, you should follow it by the corresponding number, which talks about the cutoff that you want to give for this particular potential. And I think I have chosen something like 10 or something, for just illustration purposes I have given 10.

Student: All distances in angstrom?

Professor: It is always, all distances are an angstrom. And what are the various pair styles available there is a huge list that is there right below, a huge list, the various kinds of pair interactions that you can actually specify in LAMMPS. In LJ itself if you take a look at it, you have various different types, for example if you say LJ cut coulomb cut that means you have to give, there is a there is a LJ interaction for the nuclear interactions between the atoms in addition to that it can also give coulombic interactions existing between the atoms. And you can give separate cut-offs for the LJ potential and separate cut offs for the coulombic interaction. So, in this manner you specify the pair style interaction between the atoms, or you are specifying what type of potential that you are going to use.

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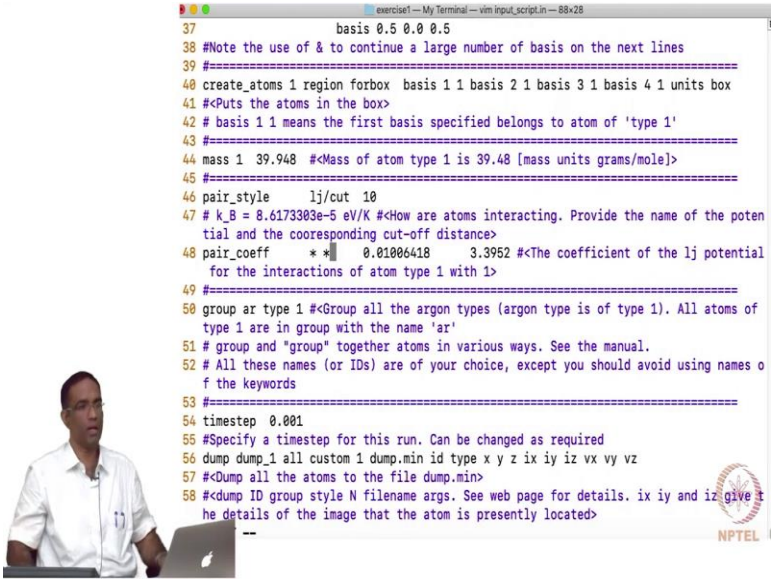

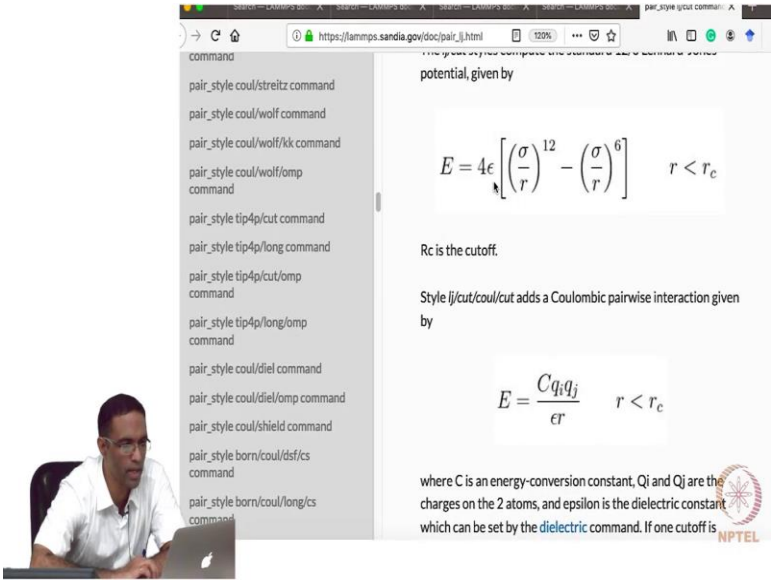

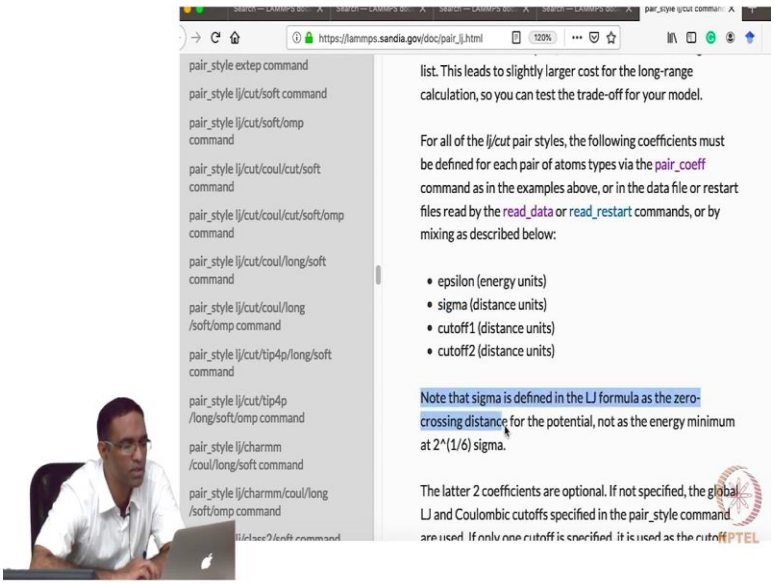
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pair_style lj/cut/tip4p /long/soft/omp command
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pair_style lj/charmm/coul/long /soft/omp command
list. This leads to slightly larger cost for the long-range calculation, so you can test the trade-off for your model.
For all of the lj/cut pair styles, the following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:
epsilon (energy units)
sigma (distance units)
cutoff1 (distance units)
cutoff2 (distance units)
Note that sigma is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum at 2^(1/6) sigma.
The latter 2 coefficients are optional. If not specified, the global LJ and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff
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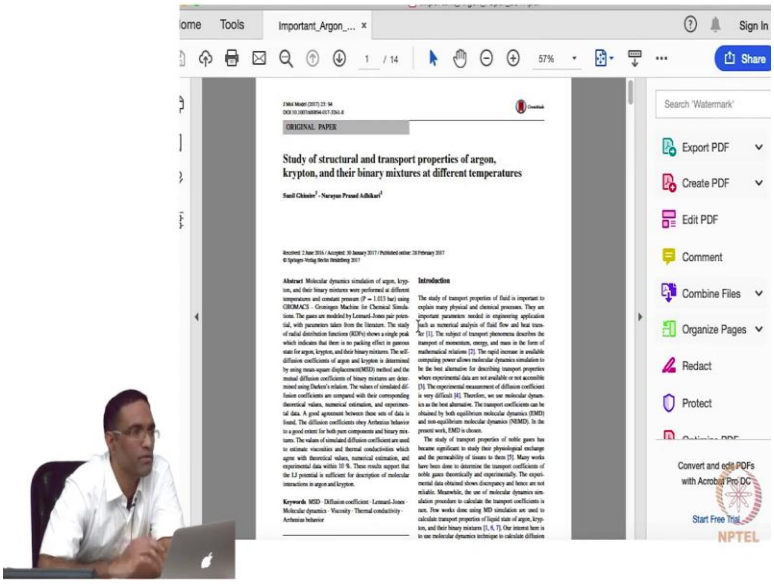
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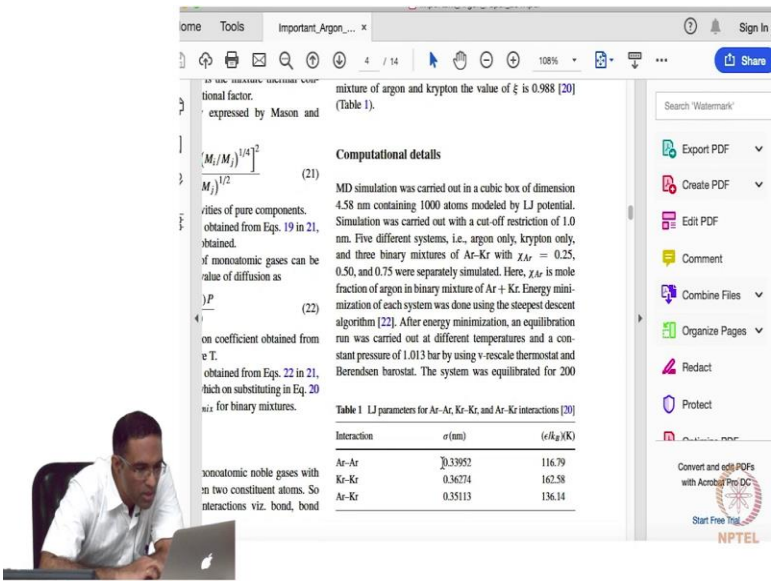
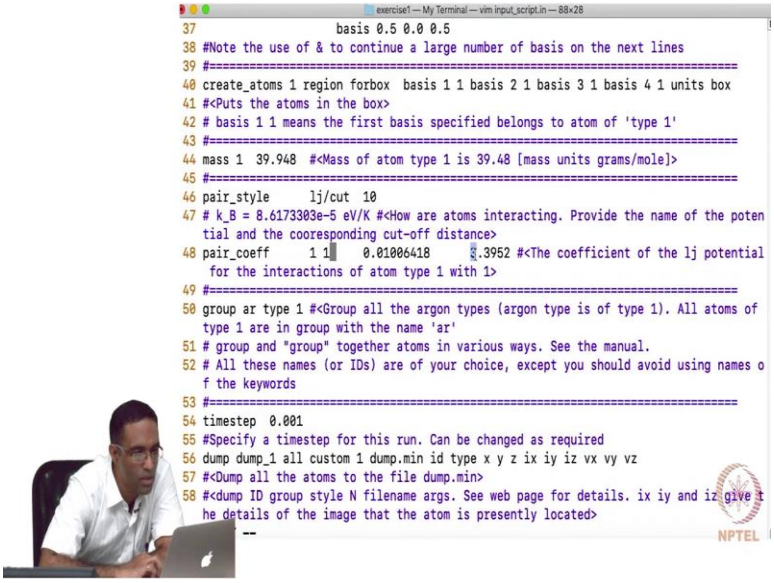
ORIGINAL PAPER
Study of structural and transport properties of argon, krypton, and their binary mixtures at different temperatures
Sunil Chhiber[2] · Narayan Prasad Adhikari[1]
Abstract
Introduction





So, next you specify for this particular pair style the coefficients. So, while you have specified that you are going to use the LJ into atomic potential, you have not yet specified what parameters you are going to use in order to model this LJ potential, basically the values of epsilon and a sigma. So, in LAMMPS, you specify the sort of interaction using this pair underscore coefficient. So, basically the coefficients for this path style interaction, and these are the atom types between which you want to have this interaction. So, 1 and 1 between 1 type, atom of type 1 and atom of type 1, you want have these interactions. So, if you have argon plus Krypton, plus xenon, each of them could be of their specific types and you could specify 1, 2 interaction and 1, 3 interaction and so on, before…

Student: In same command?

Professor: In the well you can do it in the same command, or you can do it in subsequent lines as well. I will just show you something in just a minute, you can do different things here. So, this for example if I replace this 1, with star, star, it means that for all possible pair interactions use these potentials. Then if I use something like if there are 4 different types of atoms in your system, if I do that there is some, let us, let us come to that when we do I do not want to talk about it now. So, there are different ways you can give these interactions and there are ways by which you can do is very quickly even if there are many different atom types. So, the first coefficient will essentially be the sigma value, sorry the first, first thing will be epsilon value.

So, this is the potential that we are looking at epsilon and sigma are the two things that we have to specify here. So, the epsilon value is the first thing that you specify in energy units, and is next is sigma. And right below that you see a sentence which is very important, the sigma that is defined here in LJ defined in the LJ formula is the zero crossing of the potential. So, the sigma is basically the distance at which the potential energy crosses zero, it is not the value at which the potential is actually a minima when you are specifying the value of a sigma right here. So, so and then you can specify cutoff distances for various things.

So, in this case in certain cases if you are using coulombic interaction in addition to the LJ interaction like I just mentioned you can specify cutoff separately for the LJ potential and another cutoff for the corresponding coulombic interactions. Now, you can obtain this data for argon from various places but I am actually looking at one specific paper where several of these, where a lot of analysis has been done on various different noble gases. So, I will just show you that paper, and we are going to do a lot of stuff from that paper in this class. So, this is an important paper for this class.

So, it talks about structure, study of structure and transport properties of argon krypton and their binary mixtures at different temperatures. So, it is a very good starting point to start learning some of these, some of some aspects of MD simulations with these simple materials. And you can try to reproduce some of the results that are there in this paper and I think that itself will be a very good exercise to learn these things properly. And you can find the interaction potential in this particular table right here, and they say the interaction between argon, argon sigma is given

as 0.33952 and if you observe carefully there is a value that I am using here as well, 3.3952 and that is simply because they have a different units here, in nanometers is what they have given.

But we are supposed to give in angstrom. So, that is the reason and then here you have 116.79 and it is normalized by kV. So, therefore we have to multiply this number by Kb in order to specify the value in electron volts for this epsilon. So, that is the way you specify the interaction. Now, this is a very simple interaction that we are talking about, but for more complicated interactions, it is possible that you may have to specify them through and through some other file, like for example an embedded atom potential is not given to you in this explicit form, you have to read in a table of values for the system that you are working with.

And if you are talking about more complicated systems such as the terse off potential, there are there are there is another way of defining the parameters, the more number of parameters are there and you have to specify them in the form of a table in another file which will be read by this file. So, for some potential it is possible to specify the inter-atomic, for some systems it is possible to specify the inter atomic potential parameters right here in the input script itself. So, for, for our case this information is more than enough, for argon krypton and all that. But when we talk about solids when we talk about ceramics or metals these things can change a bit.

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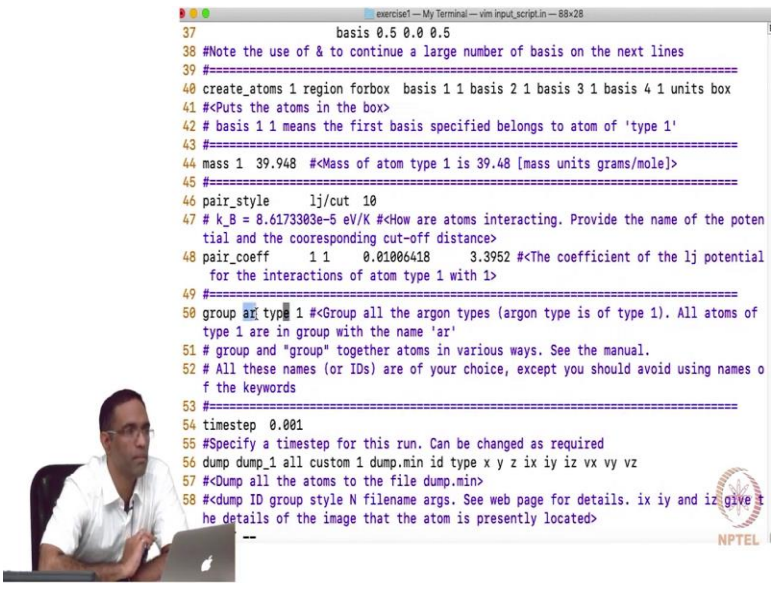

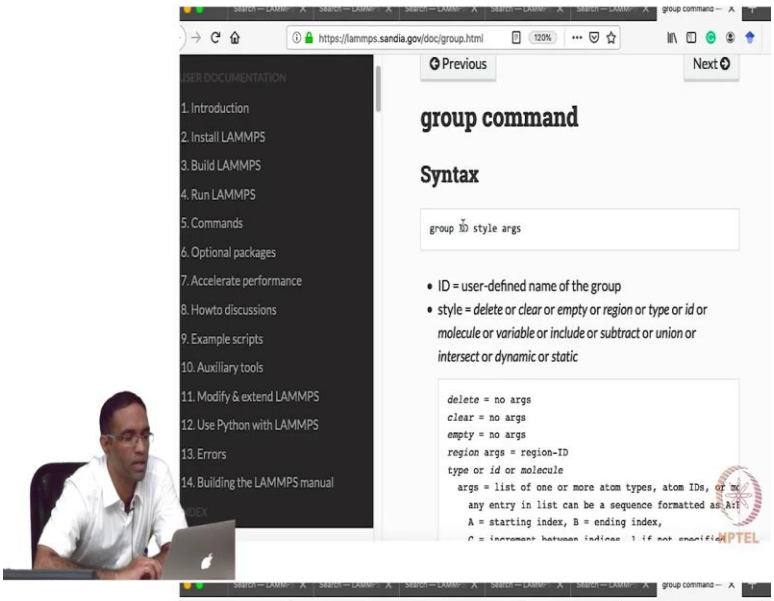
https://lammps.sandia.gov/doc/group.html
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group command
Syntax
group ID style args
• ID = user-defined name of the group
• style = delete or clear or empty or region or type or id or molecule or variable or include or subtract or union or intersect or dynamic or static
delete = no args
clear = no args
empty = no args
region args = region-ID
type or id or molecule
args = list of one or more atom types, atom IDs, or m
any entry in list can be a sequence formatted as A:I
A = starting index, B = ending index,
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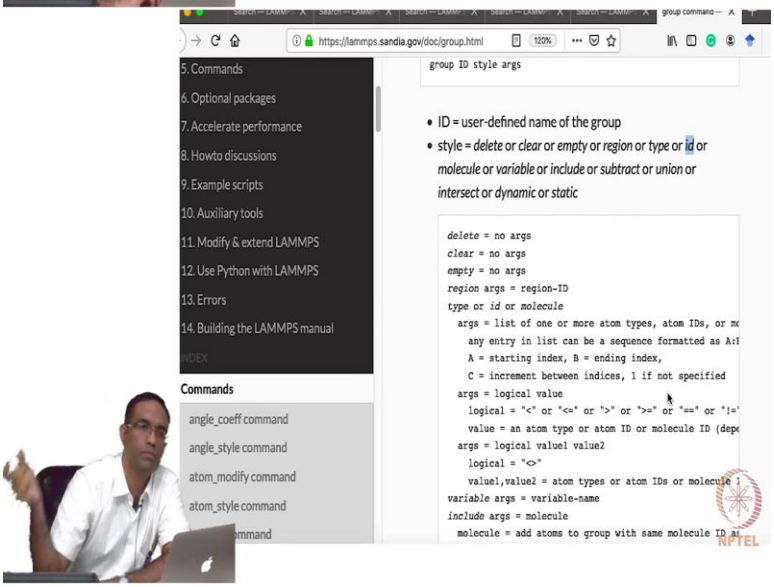
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Commands
angle_coeff command
angle_style command
atom_modify command
atom_style command
group ID style args
• ID = user-defined name of the group
• style = delete or clear or empty or region or type or id or molecule or variable or include or subtract or union or intersect or dynamic or static
delete = no args
clear = no args
empty = no args
region args = region-ID
type or id or molecule
args = list of one or more atom types, atom IDs, or m
any entry in list can be a sequence formatted as A:I
A = starting index, B = ending index,
C = increment between indices, 1 if not specified
args = logical value
logical = "<" or "<=" or ">" or ">=" or "==" or "!="
value = an atom type or atom ID or molecule ID (depe
args = logical value1 value2
logical = "<>"
value1,value2 = atom types or atom IDs or molecule I
variable args = variable-name
include args = molecule
molecule = add atoms to group with same molecule ID as
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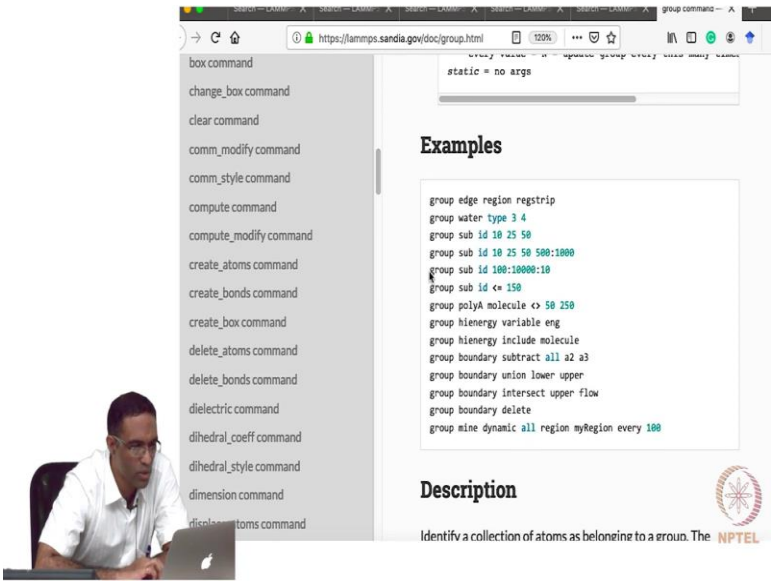

Then what I am going to do is? I am going to group all the atoms that are belonging to one particular type into some set. And you can do a lot of things with this with this group command it is it is quite powerful. So, it is a good idea to take a look at that as well, for example say you have a group, you want you want to only print out the positions and the velocities of atoms for which the x-coordinate is less than some value. Then it is possible to use the group command to put all the atom IDs with, with x-coordinate less than a certain value into a specific group. And then you know use that name that you just specified.

So, if you looked at the group, there is a name that I specified, it is called as a group ID, which is something that you give. And you can use that value ar to refer to it refer to that set of atoms, somewhere later on in the script. So, all atoms of type 1 are given this name ar, and there are different ways of actually specifying the group. So, this is the group command, this is a group this is the ID. So, ar in our case, the style, the style can be one of these, so my style was type, I am going to group the type. But you can also group it based on ID of the atom and you can use all sorts of logical operators to say if ID is greater than this and less than this, put all these atoms in a group, you can do all such things with the group command.

So, for simple cases these things might seem not so useful, but when you are doing real simulations and when you want to group certain, you can group certain set of atoms in a simulation box and run a different simulation on those atoms, when compared to the others. So, when you want to do such things, it becomes extremely useful to use this group command. So,

then so for example if you do this group sub, sub is the name of the group by ID. So, from 100 to 10,000 every 10 IDs you put it in a group. So, all these things help you actually do a lot of the post-processing right here and the input script, you may not be able to see it right now. But it is a good idea to remember this group command before doing writing any explicit code by yourself to actually do analysis.

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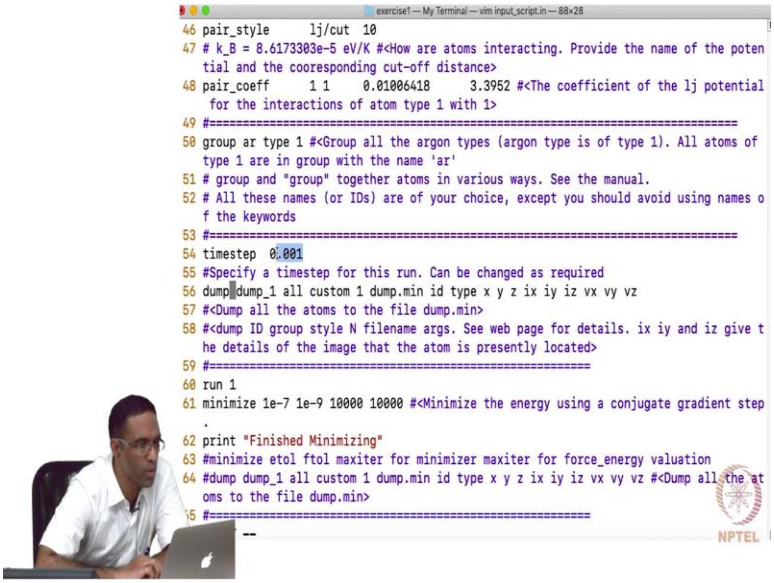

Then there is a command called time step. So, we are obviously solving these equations of motion numerically, and we have to specify a time step, and I am specifying a time step as 0.001 and what units it is? It is in Pico seconds, Pico seconds is the standard units for the units that we have chosen here, which is the metal units. So, 0.001 Pico seconds, which is 1, 2, 3, 1, femtosecond is the time step, that I am going to use. Now, this can be changed as and when you need. So, if you want to increase the time step for some other runs, you can later on specify another time step followed by the corresponding value that you want to use.

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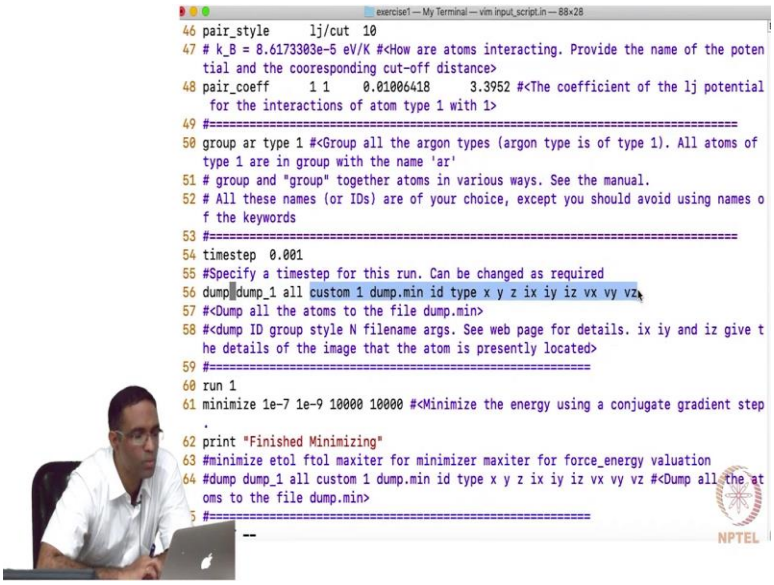

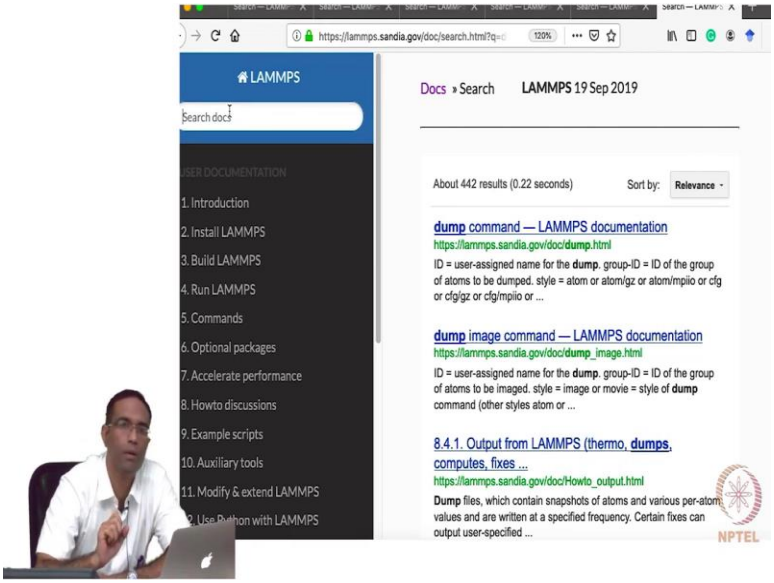

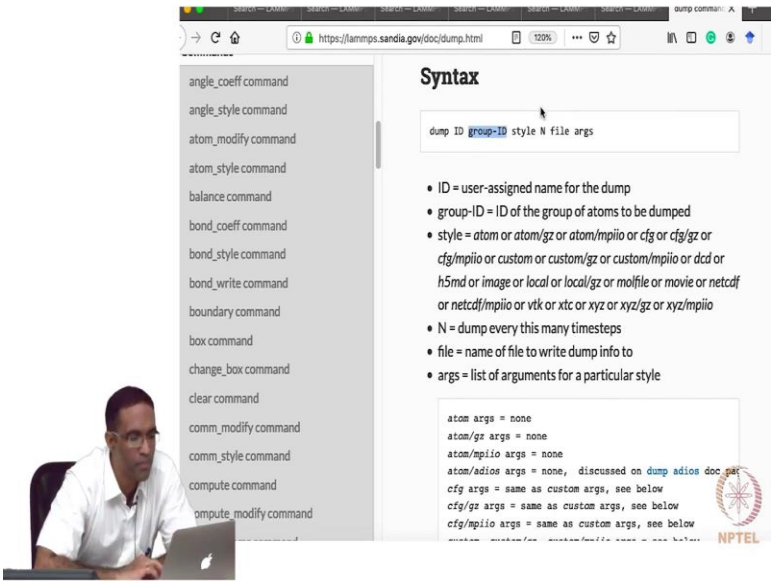

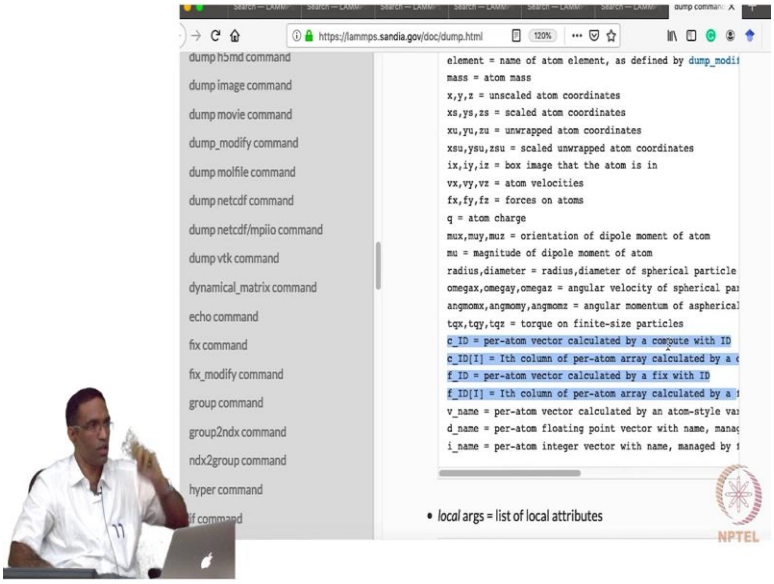

Now, this is an important command, which is dump, dump means dump the values literally. So, write the values into a output text file. Now, this is a key word this is a dump ID, if you want to refer to it at a point later on in the script, all means all the atoms in the system that is a default group that is present in LAMMPS. So, you do not have to say, you do not have to explicitly put all the atoms into a group called all, the group all already exists. So, all the atoms and then you specify the manner in which you want to print out information into a output file. So, in this, in this case I am going to use a customized, I am going to say what I want to print, I want to, I want LAMMPS to print out into a file say.

So, I use them, I use the key, I use the style custom and I say every step during the simulation print out the information, and dump underscore min is basically the file into which I want to write the information. And what information do I want to write? I want to write the ID, I want to write out the type of the atom, the x coordinate, the y coordinate, the z coordinate and then something called as ix, iy, iz, which basically is going to tell me in which periodic image my atom is actually located, for whatever reason that might be useful later on in my analysis. For example, I when we run this we will see what this means. So, right now you just understand that this is going to be either 1, 0, 0, 0, 1, 0, 0, 0, 1, and so on like that. So, it is going to tell you if this is your main box, if an atom actually had moved to this box, it is going to tell you that, the image flag for that particular atom is going to be 1 in the X direction, 0 in the Y direction, and 0 in the Z direction. So, and then vx, vy, vz, are obviously the velocities of the atoms.

Student: Sir different between dump and dump 1?

Professor: Dump 1 is a dump ID. So, everything has a ID in LAMMPS, so just like how you have group, group ID, to refer to that group somewhere later on in the file, in a similarly you have dump, dump ID. So, that you want to refer to that dump, you want to say for example dump keep dumping, but then you want to also have a line which is stop dumping information here. So, how will you refer to the dump? Through its dump ID, you say un-dump dump ID, it will stop writing information to that particular file.

Student: The actual name of the file is dump dot min?

Professor: The actual name of the file into which it puts information is the dump dot min. So, now the dump is now evolved a lot I mean a lot of things can be you can dump it in various different formats, you can dump it in a movie format, you can dump to the position of all the atoms in an image format and just take a look at the png file or the jpg file as a function of time. Previously we had to like do other things to actually take a look at it. So, this is our, the one that I am using here is the old, the old style. So, we just use dump the corresponding dump ID, what group ID you want to dump? So, basically we defined a group called ar, you remember? But now I am just putting all, but you can I can also put ar, and I will get the same information. Then what style how in what format do I want to print out the information?

So, I have chosen custom, custom and then how frequently I want to print it out N, the name of the file and the corresponding arguments, the arguments list of arguments, list of arguments for a particular style. So, if I am doing custom it can be a lot of stuff. So, it can be all these things ID, that I am printing out the corresponding x, y, z, information, the box image that the atom is in, the corresponding velocities of the atom, the corresponding forces on the atoms, charge on the atoms. And then anything else that I may have computed using something called as a compute command, all these things can be printed out and these this dump command does the job for information that is related to per atom. Whereas the thermo command does stuff that is related to the entire simulation box, for many atoms together such as the pressure, or the volume, or the temperature, and things like that.

So, there is a there are two outputs that will come out of LAMMPS, like we mentioned one as a log file and the other one is this dump file, both of each both, both of each you can control what do you want to print, and how frequently you want to print. The log file generally contains information for the entire system, whereas the dump is per atom information. So, that is the way this dump works, this thing I have given 1. But remember this is, these simulations are all for practical purposes, when they are actually used in research they are, they all run for days and months and things like that. And careful thought has to be given how frequently you want to print out information especially, especially things like the positions and the velocities of all the atoms in the system.

So, if you have a simulation, which comprises of million atoms. So, and you say and you are running it for say 10 picoseconds, and you are using a time step of one femtosecond, and you imagine if you say print every step, the x coordinate, the y coordinate, the z coordinate, the velocities of all the atoms in the system, the size of your dump will just be so large, will be, it will go to gigabytes. And it can be extremely hard for you to post process that, anyways you have to write a post processing code to read it, that itself will take a long time.

So, you have to be careful how frequently you want is information to be dump and a lot of lot of analysis has to be done to set up your input file so that it does things in an optimal manner and that can actually be a difficult task, before you run your actual simulation you might have spent a significant fraction of time and figuring out how to do it optimally for your system. So, be careful about using this number 1, be careful about using this time step, because if you give it if

you are making it extremely small, then the number for a given time you will have to run it for a larger number of steps. And, and the system may not need such a small time step. So, you have to perform several trial runs before you actually figure out what, what time steps and what how long you have to actually run your system.

Student: Sir instead of 1 times step so will it is so be ID for 5th, 10th, 15th, like that?

Professor: Yes, so, if I every, so many time steps. So, if I change this to 5, it is going to print that information every 5 time steps.

Student: So, it is start to 5 and then 10, 15.

Professor: It will start from the first one that is, it is seeing and then the 6th plus 5, 6th one,11th one, and so on.

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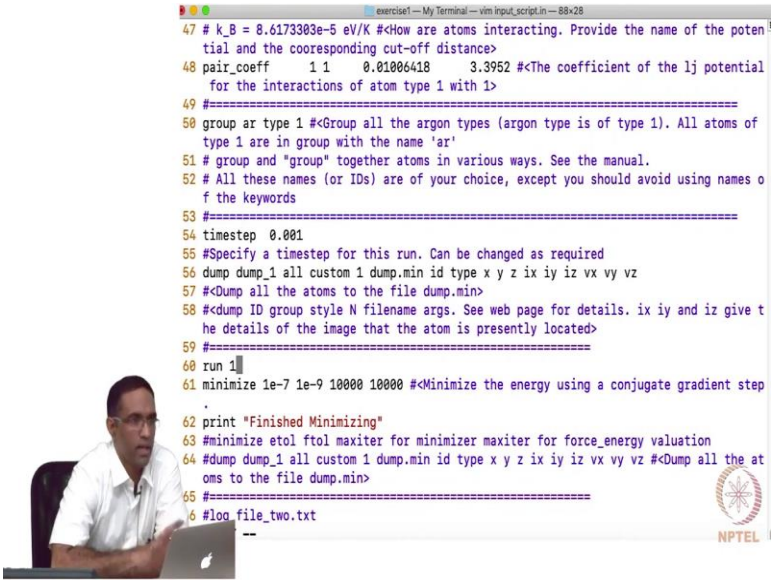

So, then I just said run 1, this is a very important command, which basically tells you how many steps do you want to run with the settings that you have just done, about this line. Right now I have not done much, what did I do, is there anything that is important here I have specified the pair style, I have specified a group, I specified a time step, and I said just dump and I just said run 1. What is it going to run is a question that that, that should be, that you should be curious about. It is not going to run anything at this point, because we have not told how the atoms are, we have not told it something that is extremely crucial yet. We come to that in a bit yeah, I just

wanted to introduce the run command, run followed by the total number of steps you want to run it.

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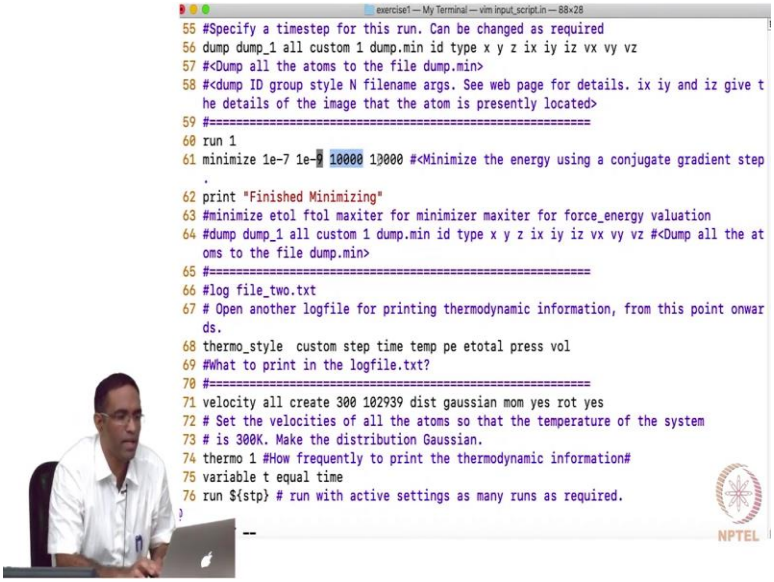
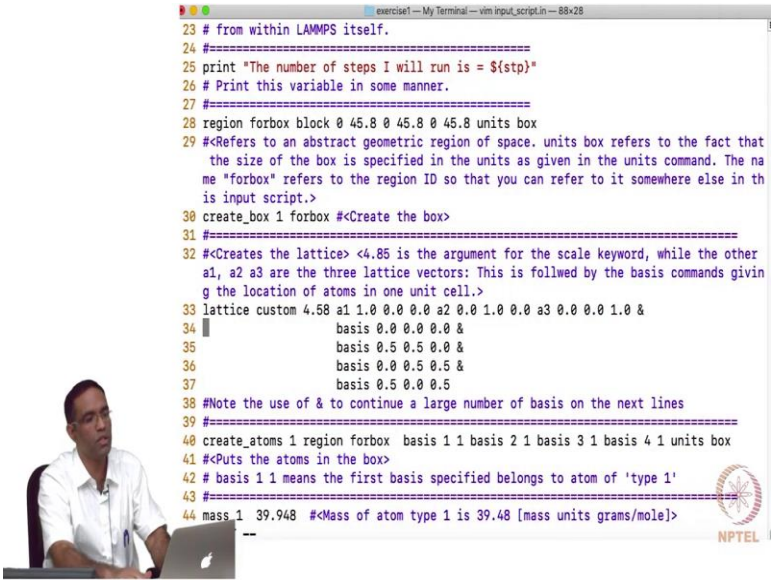


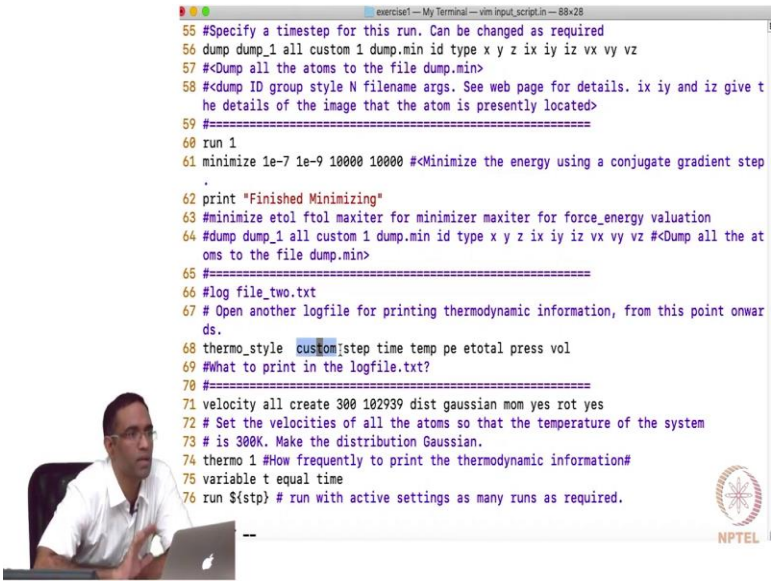


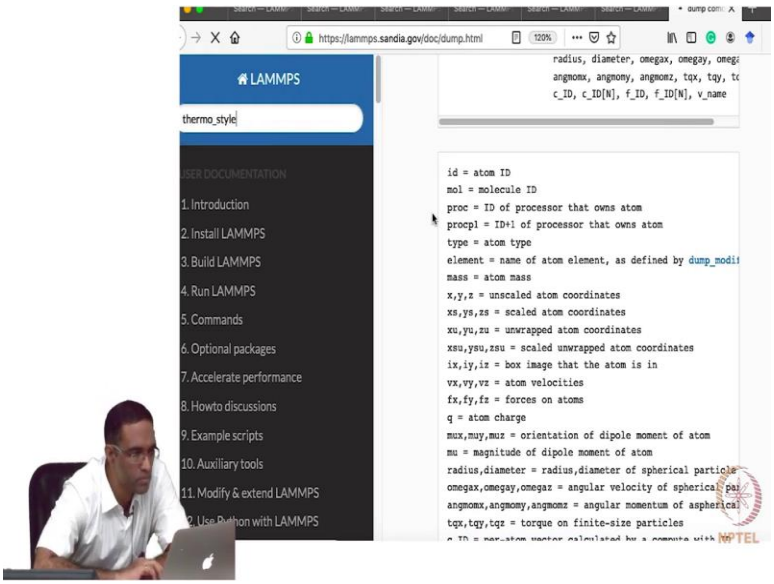
Minimize is a command that is used to actually minimize the energy of the system. So, your atoms might be for the current case I have all the atoms are placed in their equilibrium positions. So, for argon it so happens that at some low temperature the, the equilibrium lattice constant is 4.58 and it takes FCC structure. So, they are all at its they are all at their equilibrium positions, and if I do a energy minimization, there is not much is going to happen, however if you have displaced these atoms a little bit randomly, if you place these atoms a little bit randomly and

perform an energy minimization. It will just take the potential energy minimize the energy and bring the atoms to their equilibrium position so that the total force on the on each atom and total energy of the system is kind of minimized.

So, the minimize command takes in four different arguments. So, it takes in what is the, what should be the as it is minimizing it will keep calculating its energy and the forces. So, between the previous iteration and the current iteration, what do you want the difference in energies or the forces to be before I can stop performing this energy minimization. And obviously you also want to specify how many times do you want to try each of these. So, these are the number of iterations one for energy and other for force and these are the tolerances that I am willing to accept for the energy and for the force. Now, this is just a print command. So, I just said finished minimizing, you have to put it in quotes, but you can have all source of variables and other things here to guide you in your analysis.

(Refer Slide Time: 24:13)




https://lammps.sandia.gov/doc/dump.html
LAMMPS
thermo_style
1. Introduction
2. Install LAMMPS
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4. Run LAMMPS
5. Commands
6. Optional packages
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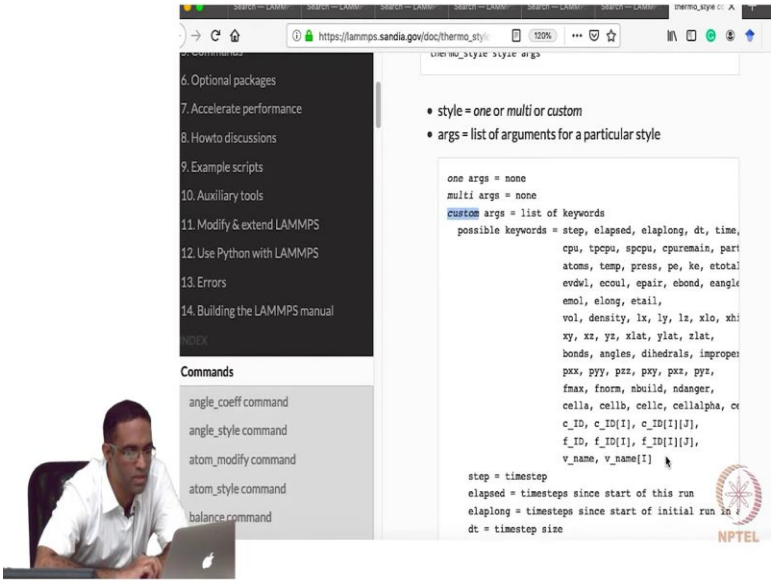
11. Modify & extend LAMMPS
id = atom ID
mol = molecule ID
proc = ID of processor that owns atom
type = atom type
mass = atom mass
x,y,z = unscaled atom coordinates
xs,ys,zs = scaled atom coordinates
xu,yu,zu = unwrapped atom coordinates
xsu,ysu,zsu = scaled unwrapped atom coordinates
ix,iy,iz = box image that the atom is in
vx,vy,vz = atom velocities
fx,fy,fz = forces on atoms
q = atom charge
mux,muy,muz = orientation of dipole moment of atom
radius,diameter = radius,diameter of spherical particle
tqx,tqy,tqz = torque on finite-size particles
NPTEL


https://lammps.sandia.gov/doc/thermo_sty
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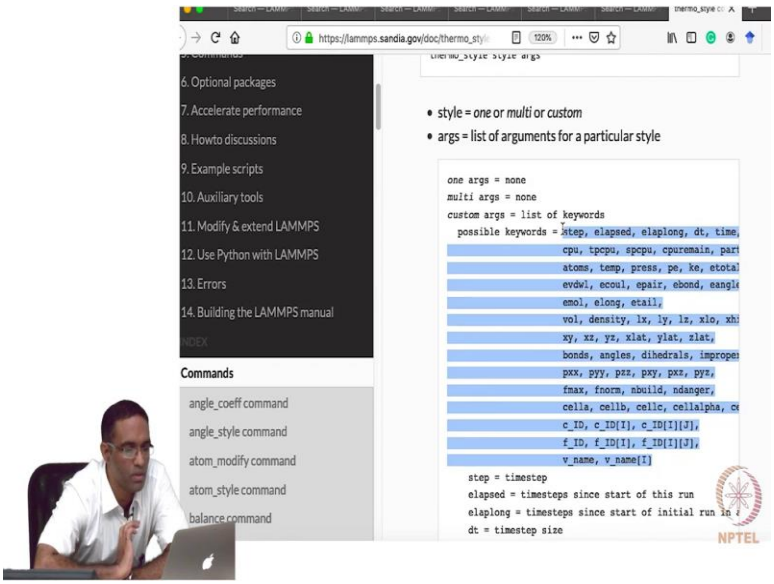
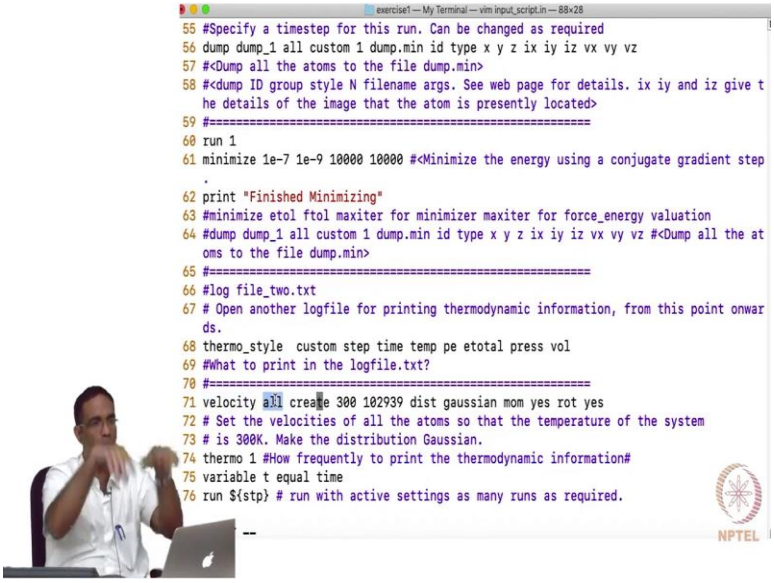
12. Use Python with LAMMPS
13. Errors
14. Building the LAMMPS manual
Commands
angle_coeff command
angle_style command
atom_modify command
atom_style command
balance command
• style = one or multi or custom
• args = list of arguments for a particular style
one args = none
multi args = none
custom args = list of keywords
possible keywords = step, elapsed, elaplong, dt, time,
step = timestep
elapsed = timesteps since start of this run
elaplong = timesteps since start of initial run
dt = timestep size
NPTEL

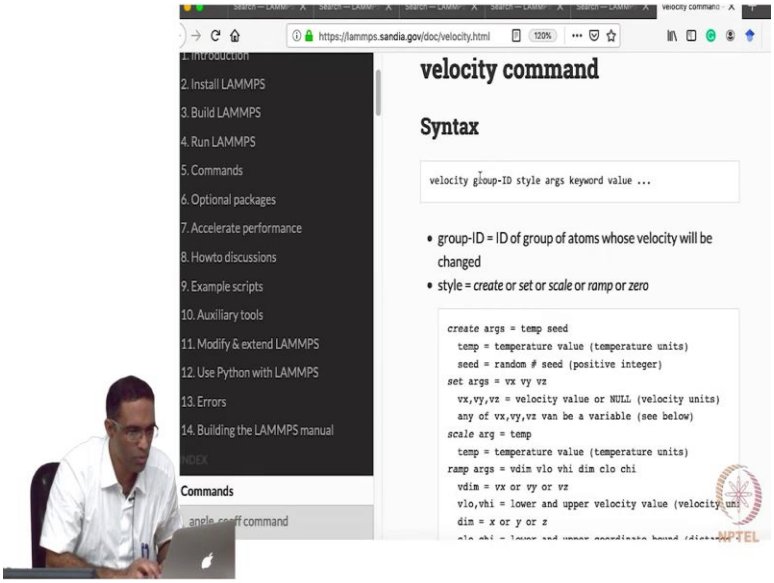


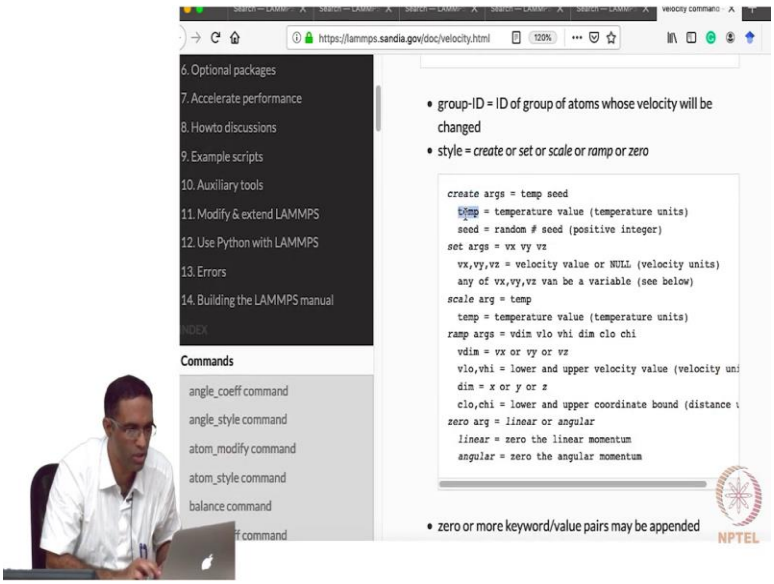
So, then is thermo style command, thermo style basically tells you the what do you want to print out in the log file. So, like I told you log file prints information of the entire system and I said custom means something that I want not the default thing that LAMMPS prints. So, that is that is what the custom style is about. So, I wanted to print the step number, I wanted to print the actual time, I wanted to print the temperature of the system, potential energy, the total energy, the pressure and the volume.

So, how do I know these keywords? So, you go to the manual, so style, custom, custom the list of keywords. So, these are the various things that you can actually print out, how much time has elapsed. Then the time step that you are using, all these things can actually be printed out. And these are the keywords that you need to use for that you cannot use something else. So, this is the precisely tells you if you want the total energy, you need to use e total right here. And all the, the, the entire list is explained what each of the short forms mean is explained right here.

(Refer Slide Time: 25:47)






https://lammps.sandia.gov/doc/velocity.html
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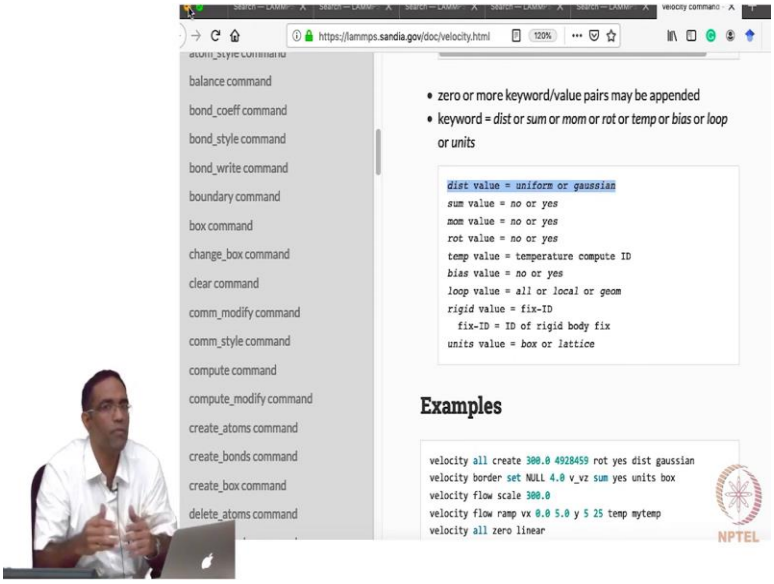
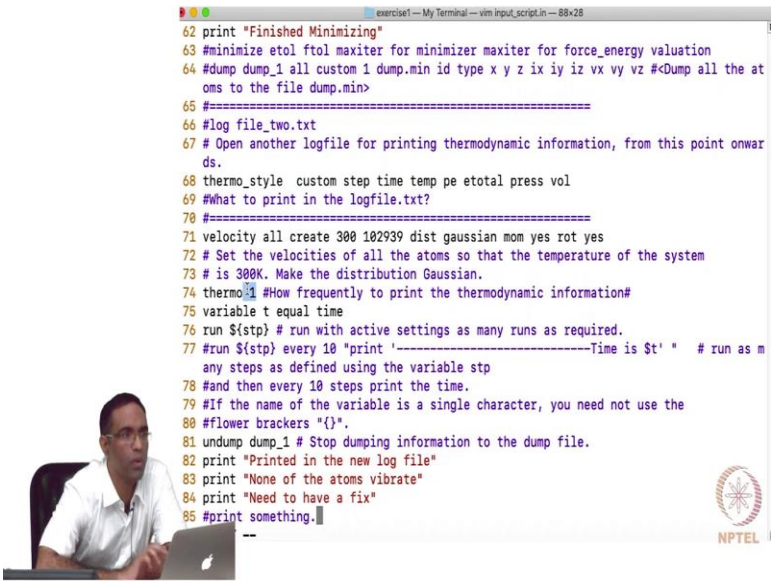
INDEX
Commands
angle_coeff command
angle_style command
atom_modify command
atom_style command
balance command
• group-ID = ID of group of atoms whose velocity will be changed
• style = create or set or scale or ramp or zero
create args = temp seed
temp = temperature value (temperature units)
seed = random # seed (positive integer)
set args = vx vy vz
vx,vy,vz = velocity value or NULL (velocity units)
any of vx,vy,vz van be a variable (see below)
scale arg = temp
temp = temperature value (temperature units)
ramp args = vdim vlo vhi dim clo chi
vdim = vx or vy or vz
vlo,vhi = lower and upper velocity value (velocity uni
dim = x or y or z
clo,chi = lower and upper coordinate bound (distance
zero arg = linear or angular
linear = zero the linear momentum
angular = zero the angular momentum
• zero or more keyword/value pairs may be appended
NPTEL


https://lammps.sandia.gov/doc/velocity.html
balance command
bond_coeff command
bond_style command
bond_write command
boundary command
box command
change_box command
clear command
comm_modify command
comm_style command
compute command
compute_modify command
create_atoms command
create_bonds command
create_box command
delete_atoms command
• zero or more keyword/value pairs may be appended
• keyword = dist or sum or mom or rot or temp or bias or loop or units
dist value = uniform or gaussian
sum value = no or yes
mom value = no or yes
rot value = no or yes
temp value = temperature compute ID
bias value = no or yes
loop value = all or local or geom
rigid value = fix-ID
fix-ID = ID of rigid body fix
units value = box or lattice
Examples
velocity all create 300.0 4928459 rot yes dist gaussian
velocity border set NULL 4.0 v_vz sum yes units box
velocity flow scale 300.0
velocity flow ramp vx 0.0 5.0 y 5 25 temp mytemp
velocity all zero linear
NPTEL



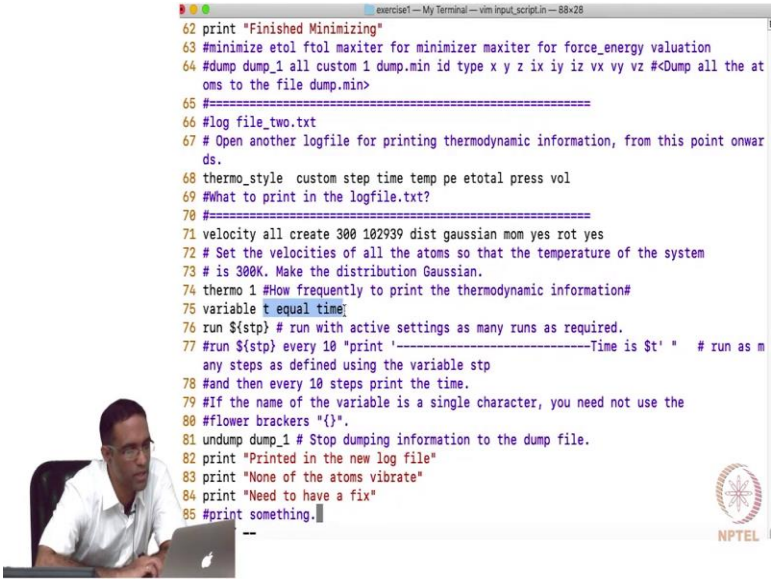
And then I want to introduce a command called velocity, in which see one of the most important things in molecular dynamics simulations is you have given the initial positions to all the atoms, because we know our crystal structure, we know the space group. So, we know the positions of all the atoms, however to start performing the integrations or integrating the equations of motion, you also need the initial velocities and it makes sense to give something that it is obviously required that you give something that makes sense. The velocities are related to the temperature.

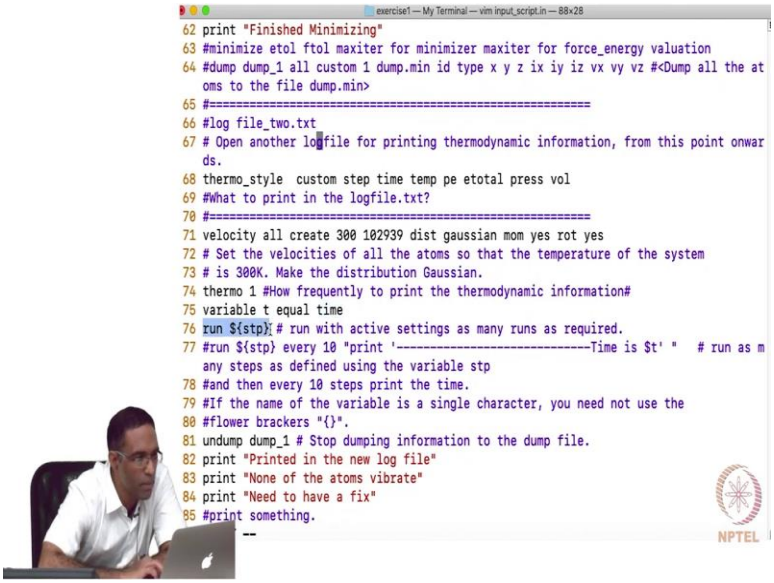
So, it is a good idea to actually assign velocities to all the atoms of the system. So, that it reflects a specific temperature. So, what I am going to do here is, I am going to say velocity for the group all that means all the atoms, create such that the temperature of the system is 300 Kelvin. And give some random seed and distribute the velocities in a Gaussian manner, this should be the velocities in a Gaussian manner. So, you should take a look at the input file, sorry velocity group ID, style args keyword value. So, create, I am going to give a temperature followed by seed, a random seed, because it is randomly going to assign the velocities in a in any some distribution that I want.

So, I am going to give it a certain distribution, the distribution is either uniform or Gaussian. I am going to give a Gaussian distribution of the velocities in the X Y and the Z directions. So, that the temperature of the system is 300 Kelvin, the instantaneous the set temperature of the system is 300 Kelvin. But it is not necessary that the equilibrium value of temperature that it

takes is going to be 300 Kelvin, different things can happen as we will see in the next example. So, this is a random seed, it can be some number, some integer.

(Refer Slide Time: 28:01)



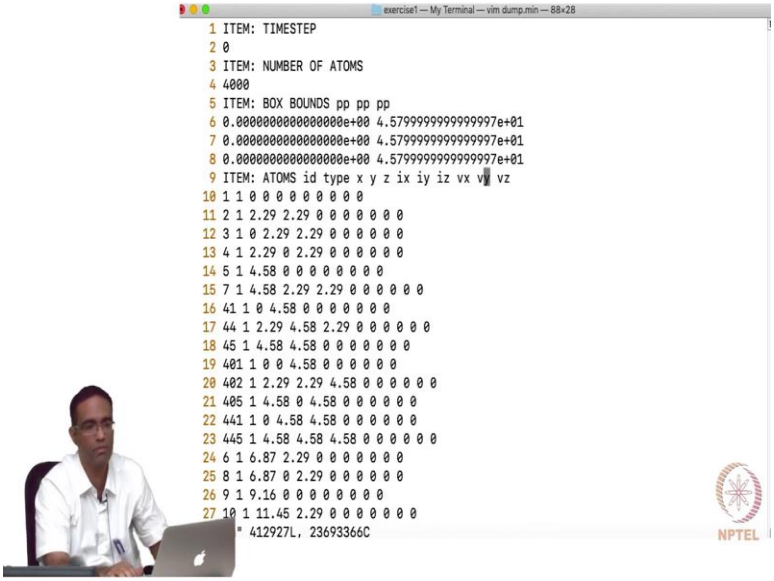


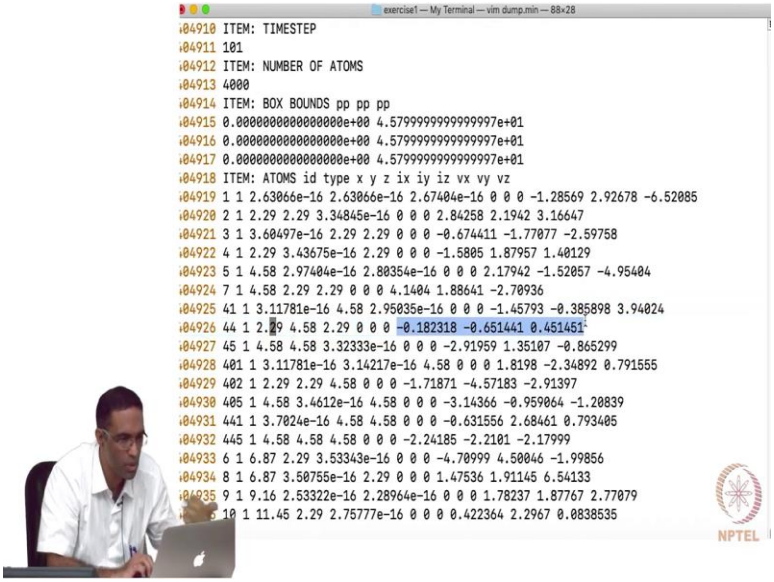
exercise1 — My Terminal — vim input_script.in — 88×28

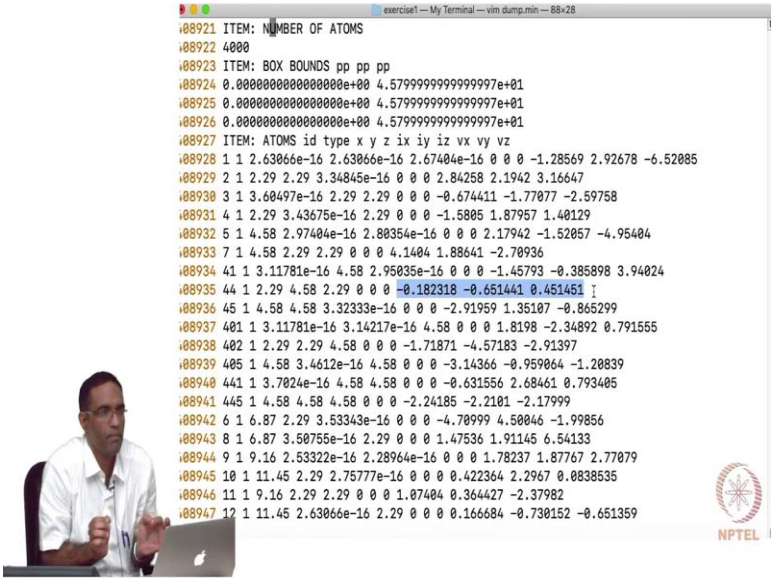
```
print "Finished Minimizing"
#minimize etol ftol maxiter for minimizer maxiter for force_energy valuation
#dump dump_1 all custom 1 dump.min id type x y z ix iy iz vx vy vz #<Dump all the at
oms to the file dump.min>
#=========================================================
#log file_two.txt
# Open another logfile for printing thermodynamic information, from this point onwar
ds.
thermo_style  custom step time temp pe etotal press vol
#What to print in the logfile.txt?
#=========================================================
velocity all create 300 102939 dist gaussian mom yes rot yes
# Set the velocities of all the atoms so that the temperature of the system
# is 300K. Make the distribution Gaussian.
thermo 1 #How frequently to print the thermodynamic information#
variable t equal time
run ${stp} # run with active settings as many runs as required.
#run ${stp} every 10 "print '-----------------------------Time is $t' "   # run as m
any steps as defined using the variable stp
#and then every 10 steps print the time.
#If the name of the variable is a single character, you need not use the
#flower brackers "{}".
undump dump_1# Stop dumping information to the dump file.
print "Printed in the new log file"
print "None of the atoms vibrate"
print "Need to have a fix"
#print something.
--
```

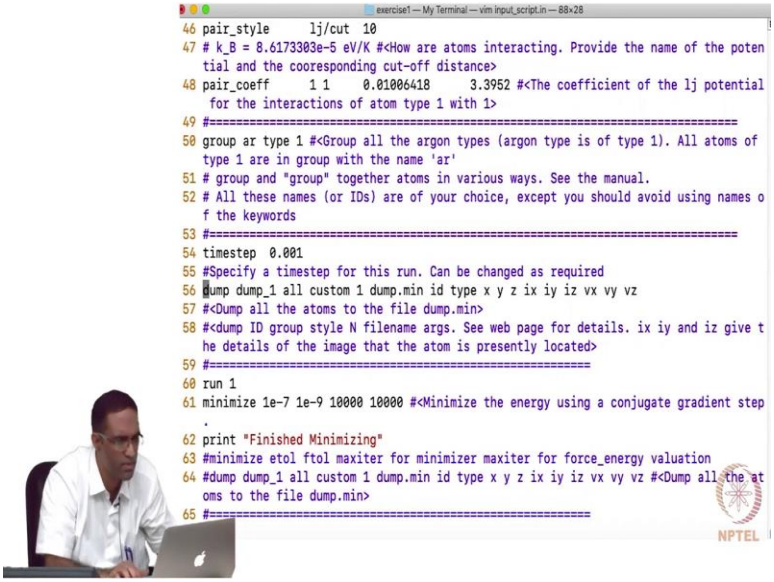
exercise1 — My Terminal — vim dump.min — 88×28

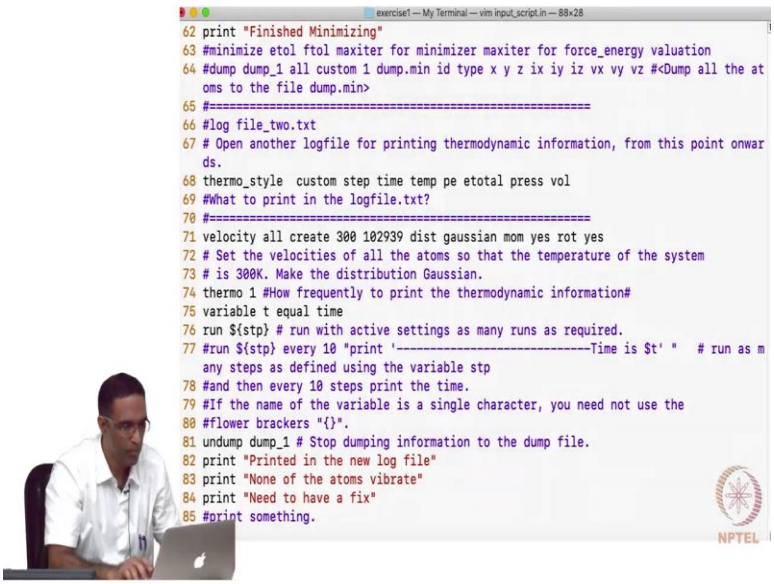
```
Aghost:    10895 ave 10895 max 10895 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Neighs:    640000 ave 640000 max 640000 min
Histogram: 1 0 0 0 0 0 0 0 0 0

Total # of neighbors = 640000
Ave neighs/atom = 160
Neighbor list builds = 0
Dangerous builds = 0
Printed in the new log file
None of the atoms vibrate
Need to have a fix
Total wall time: 0:00:03
Narasimhanhomeair:exercise1 narasimhan$ lammps < input_script.in >output.txt
Narasimhanhomeair:exercise1 narasimhan$ ls
configfile              input_script.in         logfile.txt
doxygen-bash.sed        input_script_doc.py     output.txt
dump.min                log.lammps
Narasimhanhomeair:exercise1 narasimhan$ rm -rf input_script_doc.py
Narasimhanhomeair:exercise1 narasimhan$ rm -rf doxygen-bash.sed
Narasimhanhomeair:exercise1 narasimhan$ ls
configfile      input_script.in logfile.txt
dump.min        log.lammps      output.txt
Narasimhanhomeair:exercise1 narasimhan$ rm -rf configfile
Narasimhanhomeair:exercise1 narasimhan$ ls
dump.min        input_script.in log.lammps      logfile.txt     output.txt
Narasimhanhomeair:exercise1 narasimhan$ vim dump.min
```


exercise1 — My Terminal — vim dump.min — 88×28
1 ITEM: TIMESTEP
2 0
3 ITEM: NUMBER OF ATOMS
4 4000
5 ITEM: BOX BOUNDS pp pp pp
6 0.0000000000000000e+00 4.5799999999999997e+01
7 0.0000000000000000e+00 4.5799999999999997e+01
8 0.0000000000000000e+00 4.5799999999999997e+01
9 ITEM: ATOMS id type x y z ix iy iz vx vy vz
10 1 1 0 0 0 0 0 0 0 0
11 2 1 2.29 2.29 0 0 0 0 0 0
12 3 1 0 2.29 2.29 0 0 0 0 0
13 4 1 2.29 0 2.29 0 0 0 0 0
14 5 1 4.58 0 0 0 0 0 0 0
15 7 1 4.58 2.29 2.29 0 0 0 0 0
16 41 1 0 4.58 0 0 0 0 0 0
17 44 1 2.29 4.58 2.29 0 0 0 0 0
18 45 1 4.58 4.58 0 0 0 0 0 0
19 401 1 0 0 4.58 0 0 0 0 0
20 402 1 2.29 2.29 4.58 0 0 0 0 0
21 405 1 4.58 0 4.58 0 0 0 0 0
22 441 1 0 4.58 4.58 0 0 0 0 0
23 445 1 4.58 4.58 4.58 0 0 0 0 0
24 6 1 6.87 2.29 0 0 0 0 0 0
25 8 1 6.87 0 2.29 0 0 0 0 0
26 9 1 9.16 0 0 0 0 0 0 0
27 10 1 11.45 2.29 0 0 0 0 0 0
" 412927L, 23693366C
NPTEL


exercise1 — My Terminal — vim dump.min — 88×28
04910 ITEM: TIMESTEP
04911 101
04912 ITEM: NUMBER OF ATOMS
04913 4000
04914 ITEM: BOX BOUNDS pp pp pp
04915 0.0000000000000000e+00 4.5799999999999997e+01
04916 0.0000000000000000e+00 4.5799999999999997e+01
04917 0.0000000000000000e+00 4.5799999999999997e+01
04918 ITEM: ATOMS id type x y z ix iy iz vx vy vz
04919 1 1 2.63066e-16 2.63066e-16 2.67404e-16 0 0 0 -1.28569 2.92678 -6.52085
04920 2 1 2.29 2.29 3.34845e-16 0 0 0 2.84258 2.1942 3.16647
04921 3 1 3.60497e-16 2.29 2.29 0 0 0 -0.674411 -1.77077 -2.59758
04922 4 1 2.29 3.43675e-16 2.29 0 0 0 -1.5805 1.87957 1.40129
04923 5 1 4.58 2.97404e-16 2.80354e-16 0 0 0 2.17942 -1.52057 -4.95404
04924 7 1 4.58 2.29 2.29 0 0 0 4.1404 1.88641 -2.70936
04925 41 1 3.11781e-16 4.58 2.95035e-16 0 0 0 -1.45793 -0.385898 3.94024
04926 44 1 2.29 4.58 2.29 0 0 0 -0.182318 -0.651441 0.451451
04927 45 1 4.58 4.58 3.32333e-16 0 0 0 -2.91959 1.35107 -0.865299
04928 401 1 3.11781e-16 3.14217e-16 4.58 0 0 0 1.8198 -2.34892 0.791555
04929 402 1 2.29 2.29 4.58 0 0 0 -1.71871 -4.57183 -2.91397
04930 405 1 4.58 3.4612e-16 4.58 0 0 0 -3.14366 -0.959064 -1.20839
04931 441 1 3.7024e-16 4.58 4.58 0 0 0 -0.631556 2.68461 0.793405
04932 445 1 4.58 4.58 4.58 0 0 0 -2.24185 -2.2101 -2.17999
04933 6 1 6.87 2.29 3.53343e-16 0 0 0 -4.70999 4.50046 -1.99856
04934 8 1 6.87 3.50755e-16 2.29 0 0 0 1.47536 1.91145 6.54133
04935 9 1 9.16 2.53322e-16 2.28964e-16 0 0 0 1.78237 1.87767 2.77079
10 1 11.45 2.29 2.75777e-16 0 0 0 0.422364 2.2967 0.0838535
NPTEL


exercise1 — My Terminal — vim dump.min — 88×28
ITEM: NUMBER OF ATOMS
4000
ITEM: BOX BOUNDS pp pp pp
0.00000000000000000e+00 4.57999999999997e+01
0.00000000000000000e+00 4.57999999999997e+01
0.00000000000000000e+00 4.57999999999997e+01
ITEM: ATOMS id type x y z ix iy iz vx vy vz
1 1 2.63066e-16 2.63066e-16 2.67404e-16 0 0 0 -1.28569 2.92678 -6.52085
2 1 2.29 2.29 3.34845e-16 0 0 0 2.84258 2.1942 3.16647
3 1 3.60497e-16 2.29 2.29 0 0 0 -0.674411 -1.77077 -2.59758
4 1 2.29 3.43675e-16 2.29 0 0 0 -1.5805 1.87957 1.40129
5 1 4.58 2.97404e-16 2.80354e-16 0 0 0 2.17942 -1.52057 -4.95404
7 1 4.58 2.29 2.29 0 0 0 4.1404 1.88641 -2.70936
41 1 3.11781e-16 4.58 2.95035e-16 0 0 0 -1.45793 -0.385898 3.94024
44 1 2.29 4.58 2.29 0 0 0 -0.182318 -0.651441 0.451451
45 1 4.58 4.58 3.32333e-16 0 0 0 -2.91959 1.35107 -0.865299
401 1 3.11781e-16 3.14217e-16 4.58 0 0 0 1.8198 -2.34892 0.791555
402 1 2.29 2.29 4.58 0 0 0 -1.71871 -4.57183 -2.91397
405 1 4.58 3.4612e-16 4.58 0 0 0 -3.14366 -0.959064 -1.20839
441 1 3.7024e-16 4.58 4.58 0 0 0 -0.631556 2.68461 0.793405
445 1 4.58 4.58 4.58 0 0 0 -2.24185 -2.2101 -2.17999
6 1 6.87 2.29 3.53343e-16 0 0 0 -4.70999 4.50046 -1.99856
8 1 6.87 3.50755e-16 2.29 0 0 0 1.47536 1.91145 6.54133
9 1 9.16 2.53322e-16 2.28964e-16 0 0 0 1.78237 1.87767 2.77079
10 1 11.45 2.29 2.75777e-16 0 0 0 0.422364 2.2967 0.0838535
11 1 9.16 2.29 2.29 0 0 0 1.07404 0.364427 -2.37982
12 1 11.45 2.63066e-16 2.29 0 0 0 0.166684 -0.730152 -0.651359
NPTEL


exercise1 — My Terminal — vim input_script.in — 88×28
pair_style lj/cut 10
k_B = 8.6173303e-5 eV/K #<How are atoms interacting. Provide the name of the potential and the cooresponding cut-off distance>
pair_coeff 1 1 0.01006418 3.3952 #<The coefficient of the lj potential for the interactions of atom type 1 with 1>
#===
group ar type 1 #<Group all the argon types (argon type is of type 1). All atoms of type 1 are in group with the name 'ar'
group and "group" together atoms in various ways. See the manual.
All these names (or IDs) are of your choice, except you should avoid using names of the keywords
#===
timestep 0.001
#Specify a timestep for this run. Can be changed as required
dump dump_1 all custom 1 dump.min id type x y z ix iy iz vx vy vz
#<Dump all the atoms to the file dump.min>
#<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>
#===
run 1
minimize 1e-7 1e-9 10000 10000 #<Minimize the energy using a conjugate gradient step.
print "Finished Minimizing"
#minimize etol ftol maxiter for minimizer maxiter for force_energy valuation
#dump dump_1 all custom 1 dump.min id type x y z ix iy iz vx vy vz #<Dump all the atoms to the file dump.min>
#===
NPTEL



So, I am going to print the thermo information every step. So, thermo 1 tells that, I am going to print the thermo information every step. And then I am going to define arbitrarily another variable just, just for the heck of it variable t equals time means, this time this time is actually a LAMMPS keyword telling me the time, for example I used that word here, to print out the time, I am just using that here. And I can print it out if I want, then I say run dollar step and step was actually a variable that was defined way before. And I said variable step equal 100 and if I see here I am going to say run dollar step.

So, you can you can imagine that this number of steps that you are going to run can be altered based on various formula depending upon your time step, or how long in reality you, you want to actually run the simulation. So, run dollar step will run it for how many steps? Right now 100 steps. And then I stop dumping to this file and then I print some information I just print some information. So, let us see what happens when I run this file, are there any questions on these basic commands?

Student: Variable is a keyword ?

Professor: Which one?

Student: Variable.

Professor: Yeah.

Student: If that we can define many things, right?

Professor: We can define many things yes.

Student: Just like python or something?

Professor: No, no, no it is not like it is not like that. So, this command says that say for example if you look at this command it says that STP is a variable, which is equal to 100 that is all.

Student: I can use STP, other STP?

Professor: You can use STP in other places like this. Now, this is a variable of type equal, this equal is actually a LAMMPS option. Now, there are several other things that are available, there is a loop variable. Then there is a Python variable, which means whatever is coming after it can be a Python code that you can run, all that all that is also possible here.

Student: All these calculations are run at…

Professor: That is the only command, no there are many other ways to this is, this is not doing much now, the what this is doing now is, it is changing the velocities of, it is giving velocities to each and every atoms of the atom in the system, such that the average temperature of the system is 300 Kelvin, the solid is doing.

Student: Everything is calculated in for this?

Professor: For the, at that instant at that when it starts.

Student: At what temperature the energy is calculated for this?

Professor: At what temperature the energy is calculated for this? At the instant, for the instance that I gave it should be 300 Kelvin.

Student: Would as the velocity is evolved with time, the temperature of the system will change?

Professor: Yes, exactly, but you will see here that is what I think you are just going a little bit ahead. So, I will run this and we will see what happens, I am running it. So, I am going to give the input script dot in. So, it is running, it ran and it is done, unfortunately not all practical

simulations can be done so quickly. So, it prints out something, it is printing out something it is this is the same information that it will print out even in the log file.

So, it is a good idea to actually redirect that to a output file, if you know Linux then you know what it means to redirect the output of command to an output file. It is done then you do not have these things running in your screen, especially when you are running longs, longs simulations. Now, let us take a look at the following things your LAMMPS file, this is the input script. So, these are the only things that will actually remain in your folder, the dump min which is basically the file that the dump is printing out. The log file which is basically the log file, which we have defined inside the input script, we said log space, log file dot txt. So, write down that all the log information in the log file. And then output dot txt is just the redirect of the, the command.

Now, let us take a look at maybe dump dot min first. So, the dump dot min looks like this. So, it says that the time step is 0, number of atoms is 4000, the box bounds that means xlo, xhi, ylo, yhi, zlo, zhi, is between 4 and 4.58, which is what we have given there 45.8. You remember we gave 0 to 45.8, 0 to 45.8, that is what is reflected here and then atoms, ID that is this is the atom ID the first one is atom ID, then is atom type, the x coordinate, the y coordinate, the z coordinate. Then the image flag in which that particular atom is located. And the corresponding velocities of that atom. Now, first you see all are zeros, because that is the first dump min did not the velocity was not set that time, then…

Student: If we do not give velocity command will it assume something or we are supposed to…

Professor: No, no it will not assume, it will assume 0, if you do not want to give velocities, this is not a valid sensible input file to do anything practical, this is an input file to introduce commands. The next input file that will, that I will talk about will run some simulations. Now, by now you should have realized that something weird is happening. So, I what is happening is all of you will expect that the atoms are actually now vibrating, when I ran it, I ran it 100 steps, we are expecting the atoms to actually vibrate, I gave it some initial velocity. But so, so let me complete going through the dump file.

So, the dump file after some time begins to have values for the corresponding velocities, because we have initialized it for some velocity and all these numbers will be exactly the same, for example in step number, this is step number 101, the atom ID 44 is having some weird velocity

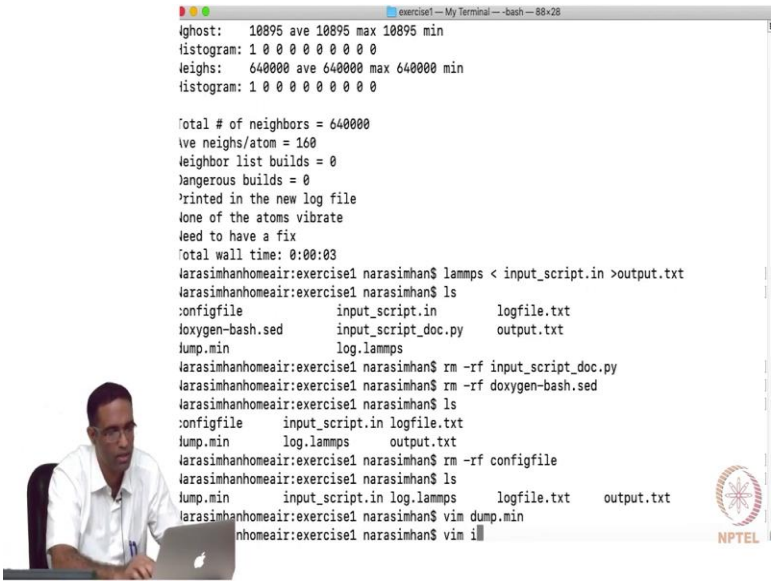
here. If you look at the subsequent step also it should have only the same velocity. So, 44 so just try to keep, just try to remember this patterns I mean I cannot, you cannot remember this, a 0.18, 0.65 and 0.45. So, if you go to the next step exactly the same value, from the time it started to now it is having actually the exactly the same value. And when did it start it started when I defined the velocity and then after that after that instance only the dump will now contain the velocity, until then although a dump was defined before say dump was defined where?

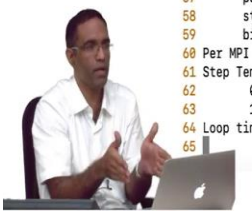
Student: After that one.

Professor: It was defined here, no it was defined here, time step dump I think that is where I define the dump. But the velocity is defined here. So, until here it is just going to print whatever velocity it has, but after this it is going to continue to append the information with that velocity information. So, keep that in mind, so although that dump is defined there and the velocities are defined here, the run is defined now.

So, this dump is going to still that dump on tag is still there. So, it is whatever for whatever settings I have done before the run all that is going to be execute it, if you do not want to be execute it, you should stop, you should use some command to stop it, just keep that in mind. So, that is what the dump file will contain and usually we use that to post process our results, look at the atoms which I will show you in a bit.

(Refer Slide Time: 37:38)



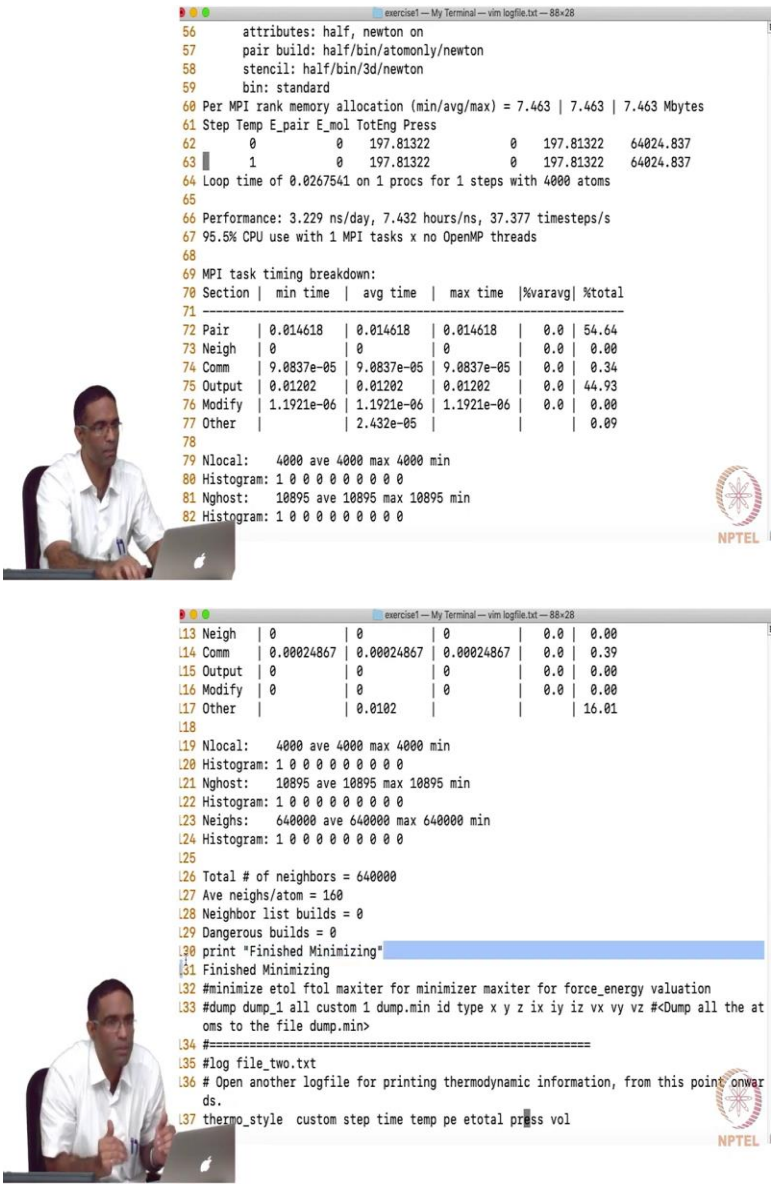


exercise1 — My Terminal — vim logfile.txt — 88×28

```
timestep  0.001
#Specify a timestep for this run. Can be changed as required
dump dump_1 all custom 1 dump.min id type x y z ix iy iz vx vy vz
#<Dump all the atoms to the file dump.min>
#<dump ID group style N filename args. See web page for details. ix iy and iz give t
he details of the image that the atom is presently located>
#=========================================================
run 1
WARNING: No fixes defined, atoms won't move (src/verlet.cpp:52)
Neighbor list info ...
  update every 1 steps, delay 10 steps, check yes
  max neighbors/atom: 2000, page size: 100000
  master list distance cutoff = 12
  ghost atom cutoff = 12
  binsize = 6, bins = 8 8 8
  1 neighbor lists, perpetual/occasional/extra = 1 0 0
  (1) pair lj/cut, perpetual
      attributes: half, newton on
      pair build: half/bin/atomonly/newton
      stencil: half/bin/3d/newton
      bin: standard
Per MPI rank memory allocation (min/avg/max) = 7.463 | 7.463 | 7.463 Mbytes
Step Temp E_pair E_mol TotEng Press
       0            0    197.81322            0    197.81322    64024.837
       1            0    197.81322            0    197.81322    64024.837
Loop time of 0.0267541 on 1 procs for 1 steps with 4000 atoms

```

exercise1 — My Terminal — vim logfile.txt — 88×28

```
Total # of neighbors = 640000
Ave neighs/atom = 160
Neighbor list builds = 0
Dangerous builds = 0
minimize 1e-7 1e-9 10000 10000 #<Minimize the energy using a conjugate gradient step
.
WARNING: Using 'neigh_modify every 1 delay 0 check yes' setting during minimization
(src/min.cpp:168)
Per MPI rank memory allocation (min/avg/max) = 8.588 | 8.588 | 8.588 Mbytes
Step Temp E_pair E_mol TotEng Press
       1            0    197.81322            0    197.81322    64024.837
       2            0    197.81322            0    197.81322    64024.837
Loop time of 0.063709 on 1 procs for 1 steps with 4000 atoms

95.1% CPU use with 1 MPI tasks x no OpenMP threads

Minimization stats:
  Stopping criterion = energy tolerance
  Energy initial, next-to-last, final =
         197.813215515      197.813215515      197.813215515
  Force two-norm initial, final = 2.96827e-13 2.94801e-13
  Force max component initial, final = 6.56948e-15 6.56948e-15
  Final line search alpha, max atom move = 1 6.56948e-15
  Iterations, force evaluations = 1 2

MPI task timing breakdown:
Section |  min time  |  avg time  |  max time  |%varavg| %total
```



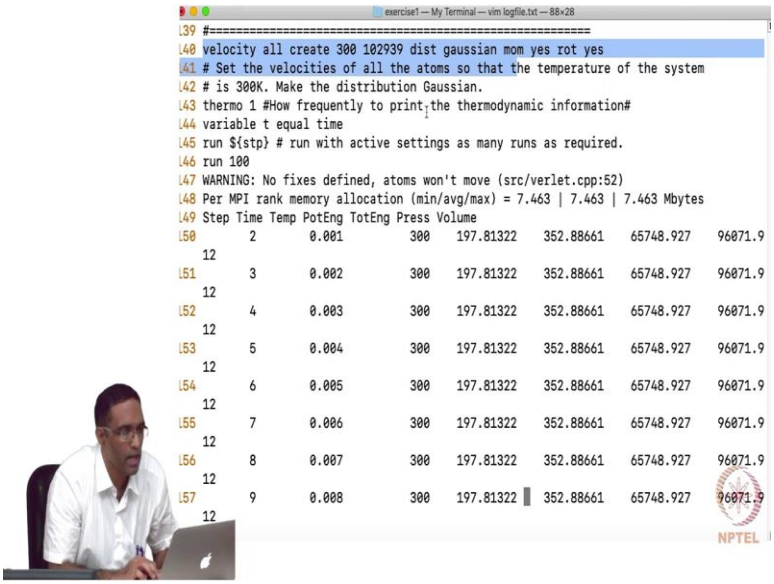
Then the log file dot txt will first contain actually the input script itself. And then you see a warning here which is the most important warning you do not have a fix defined. So, your atoms will not move, it will not move. So, and then you have the first whenever you are seeing a step command, then it essentially means that you have printed out some thermodynamic information there. So, the thermodynamic information that we have asked it to print is here time, temperature, potential energy, total energy, pressure volume. This step that it is printing out is for the minimization step that we requested, remember we asked to do some minimization.

So, this is the step where it is trying to minimize, it is by default plotting the pair potential energy, the molecule energy, and the total energy, and the pressure of the system. And then it is

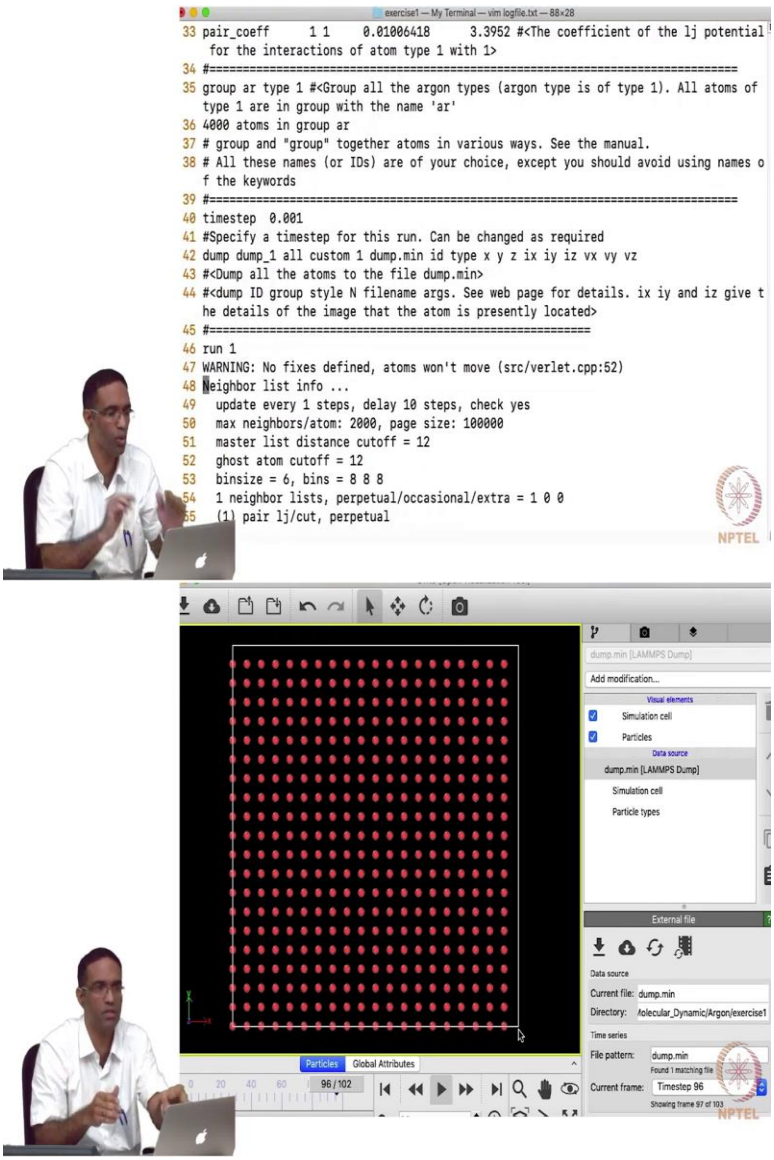
going to talk about what is the stopping criterion, the energy tolerance and all the info information that you have given. And then the final value that it got. So, the based on the force the initial and the final arc 2.96827 e to the minus 13 and 2.94801 e to the minus 13.

So, they both are apparently differing, only by the amount that we have requested. So, it is talked, similarly the values of the energies are also given here, that pretty small. And then there is actually a this stopping criterion is energy tolerance. So, which means that it stopped based on your energy tolerance criteria rather than force tolerance or the number of iterations that you have given. Because minimize consistent of what it consisted of the tolerance for the energy, tolerance for the force, number of iterations for the energy, number of iterations for the force. So, it is telling you on what criteria I actually stopped minimizing the function. So, this is the first part where some output is written concerning your simulation. So, it is finished doing that, it says finished minimizing is something that we have printed out after the minimize command. So, it is printing it out here print finished minimizing, finished minimizing.

(Refer Slide Time: 40:18)



```
# is 300K. Make the distribution Gaussian.
thermo 1 #How frequently to print the thermodynamic information#
variable t equal time
run ${stp} # run with active settings as many runs as required.
run 100
WARNING: No fixes defined, atoms won't move (src/verlet.cpp:52)
Per MPI rank memory allocation (min/avg/max) = 7.463 | 7.463 | 7.463 Mbytes
Step Time Temp PotEng TotEng Press Volume
0       2       0.001         300    197.81322    352.88661    65748.927    96071.912
1       3       0.002         300    197.81322    352.88661    65748.927    96071.912
2       4       0.003         300    197.81322    352.88661    65748.927    96071.912
3       5       0.004         300    197.81322    352.88661    65748.927    96071.912
4       6       0.005         300    197.81322    352.88661    65748.927    96071.912
5       7       0.006         300    197.81322    352.88661    65748.927    96071.912
6       8       0.007         300    197.81322    352.88661    65748.927    96071.912
7       9       0.008         300    197.81322    352.88661    65748.927    96071.912
8      10       0.009         300    197.81322    352.88661    65748.927    96071.912
9      11        0.01         300    197.81322    352.88661    65748.927    96071.912
```



Then I am starting to do I set the initial velocities, and then I am running 100 steps. And this is the information that it is actually printing out for the 100 steps, it gives you the first line of before this table it tells you the step the time, the temperature of the system, the potential energy, the total energy, pressure, volume. So, the temperature is 300 exact, for all the 100 steps every step temperature is exactly 300 and potential energy, total energy, pressure, volume are all 100. It is calculating the pressure and all volume is obviously the volume of the simulation box. This is the content of the log file and these are the files that you will often need in order to achieve your simulation, simulation is going to make sense.

Student: Sir in this input file initially defined by dump command?

Professor: Yes.

Student: How? We did not told it to start running it?

Professor: We gave a run 1 you see you gave a run 1.

Student: Sir for this the velocity profile will be ?

Professor: 0 the velocities are 0. So, the first dump, the first velocities are all 0.

Student: Sir the velocity command was not there in input. The command is not same.

Professor: Even the last, in the in the input script that I gave you the velocity command is not there. So, it will be 0 always, but in the command since I modify this morning and I had a velocity command to actually I chose to explain this today so that is why it is you do not have, why do not you add the velocity command, this is coming now, if you add a velocity command is running. Why do not you all add a velocity command and run the simulation?

Student: So if we wrote one the body to have any velocity as a whole, the center of mass of the system should remain…

Professor: Fixed.

Student: We have to insure that.

Professor: Yes.

Student: So if we do not give that mo ms command, the velocities of the atoms may evolve with time and simultaneously with center of mass may also start moving.

Professor: It could happen, it could happen but in this case we are just giving the velocity for one instance, we have not yet evolved it, because like I mentioned, I do not have an integrator, yes that is an important step.

Student: Something is there.

Professor: Something is wrong?

Student: Something is coming, means non 0.

Professor: That is all you can check, you can, otherwise you will have to now perform the calculation to see if it is 300, we can trust that it will be 3, it will correspond to a 300 Kelvin temperature only.

Student: Sir is it sampling some Gaussian curve?

Professor: Yes, because you said dist Gaussian. In the current exercise if you looked at the log file, you see that there is a warning it says that no fixes are defined atoms would not move. So, even though you have prescribed initial velocities and initial positions, if I looked at the atoms in say Ovito I will show you that maybe for today, which is a simple thing to do. So, let us open Ovito, and then let us just drag and drop our dump min here, a drag-and-drop dump min here on the lower right hand side you can see that this Ovito is actually reading each and every frame that is actually being printed out to the dump file.

So, it is basically reading the, the positions of all the atoms, that is in the system and this is our actual system, this is the system that was created by the lattice command and you are printing out all the positions and the velocities and all that and you can see there is a little bit of gap here, not to worry there is not anything serious. It is just that if you repeat this in the right-hand side on the top it basically is going to repeat as a periodic image. So, you should not have an atom at the lower right hand side corner, if you do that it means you are overlapping two atoms. Please remember that there is always this gap will appear, it is not wrong. It leads all this and then you can play it and then look at how atoms are moving if at all they move in this case they are not going to move.

But the main reason as to why that is happening is although we defined initial positions and velocities, you did not start integrating the equations of motion. We need to perform an integration of the equations of motion, the specific initial velocities, initial positions is not going to do anything. So, the first integrator that we will learn is an NVE integrator, it is just a simple solution of the Newton's equations of motion and it will update the positions and velocities as a function of time. So, we will do that in the next class.