Functional of Computational Materials Modelling
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Department of Mechanical Engineering
Indian Institute of Technology, Madras
LAMMPS Exercises - 2

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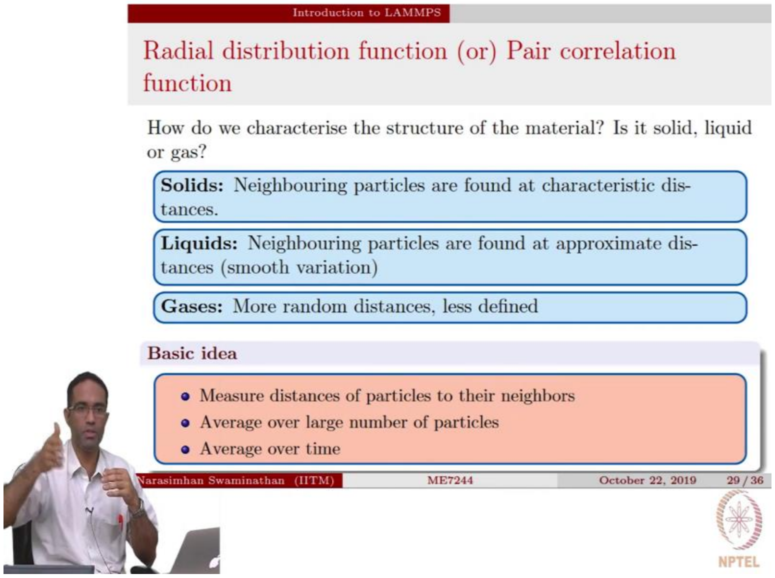

Introduction to LAMMPS

Radial distribution function (or) Pair correlation function

How do we characterise the structure of the material? Is it solid, liquid or gas?

Solids: Neighbouring particles are found at characteristic distances.

Liquids: Neighbouring particles are found at approximate distances (smooth variation)

Gases: More random distances, less defined

Basic idea

- Measure distances of particles to their neighbors
- Average over large number of particles
- Average over time

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Good Afternoon. So, let us look at another property that is important for materials or it is important to actually analyze the structure of materials and it is called as the radial distribution function or the pair correlation function. So, essentially is a reflection of the underlying order that is there in the material, for example, if you have a solid it has long range order and if you have liquids it has short range order only. So, we will, we will actually take a look at what this exactly means and how it is actually calculated using LAMMPS. So, this is demonstrated so as to show how you can actually calculate properties in LAMMPS which are not per atom, but for the entire system, this is for the entire system.

So, if you consider a solid, all the atoms are arranged in a periodic manner. So if you sit on any atom and start going away from that atom, for some distance, you are not going to find any atoms, any new atoms. But suddenly at a particular point at a specific distance, you will start seeing a certain number of atoms where that is basically the first nearest neighbor to that atom. Then if you continue going further, apart from that, again, you will not see any atom until you reach a next distance. In that manner, if you keep going further and further, you will start seeing atoms at specific distances only.

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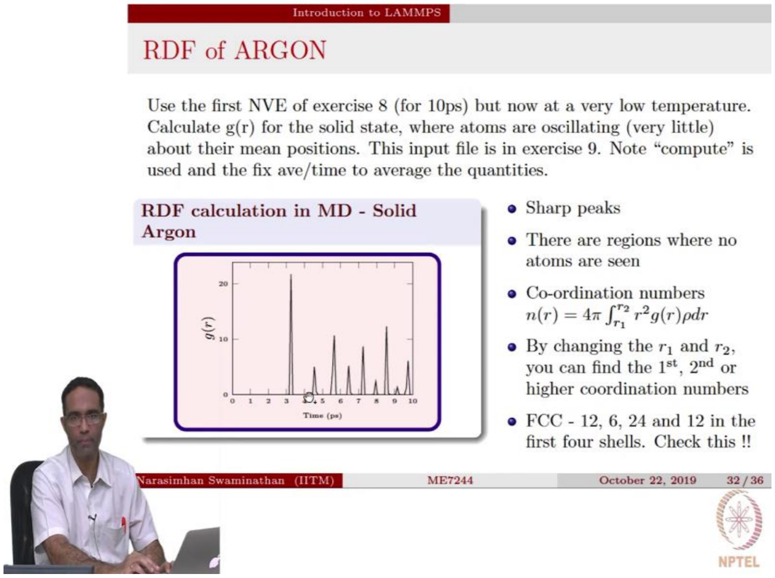

RDF of ARGON

Use the first NVE of exercise 8 (for 10ps) but now at a very low temperature. Calculate g(r) for the solid state, where atoms are oscillating (very little) about their mean positions. This input file is in exercise 9. Note “compute” is used and the fix ave/time to average the quantities.

RDF calculation in MD - Solid Argon

- Sharp peaks
- There are regions where no atoms are seen
- Co-ordination numbers $n(r) = 4\pi \int_{r_1}^{r_2} r^2 g(r) \rho dr$
- By changing the r_1 and r_2, you can find the 1st, 2nd or higher coordination numbers
- FCC - 12, 6, 24 and 12 in the first four shells. Check this !!

So, if something like that happens, then it basically characterizes a solid, so something like this. So, this is basically telling you that the probability of finding an atom at this distance from a given atom, so say you are sitting at 0, the coordinate is 0 and as you start going away from the center of the atom, all of a sudden at this particular distance, you will see a large number of atoms. Then again you see no atoms, you see a certain number of atoms. And this continues, if you see a radial distribution function that looks like this, it is basically a solid.

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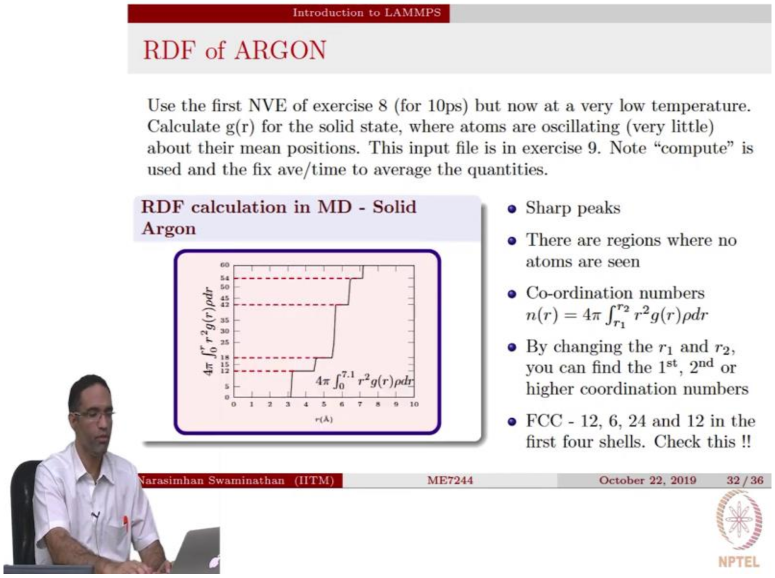

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And for liquid, it is going to look something like this.

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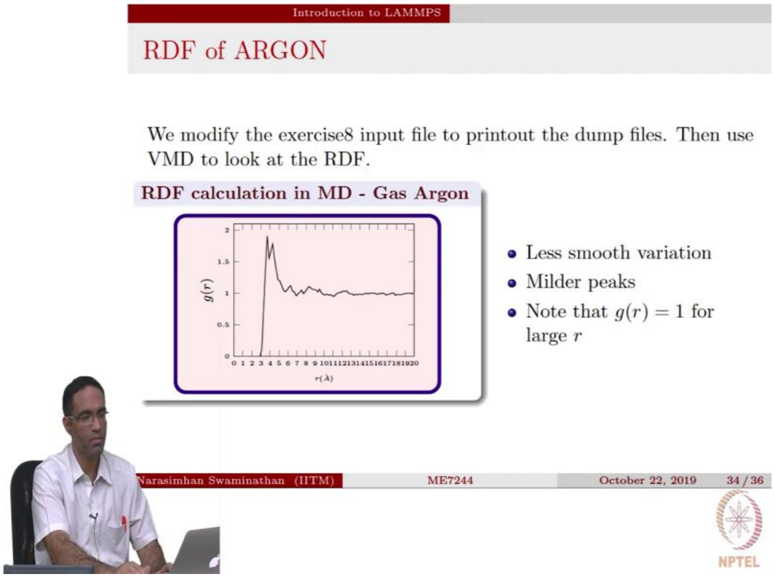

Introduction to LAMMPS

RDF of ARGON

We modify the exercise8 input file to printout the dump files. Then use VMD to look at the RDF.

RDF calculation in MD - Gas Argon

- Less smooth variation
- Milder peaks
- Note that $g(r) = 1$ for large r

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And for gas, it is going to look something like this.

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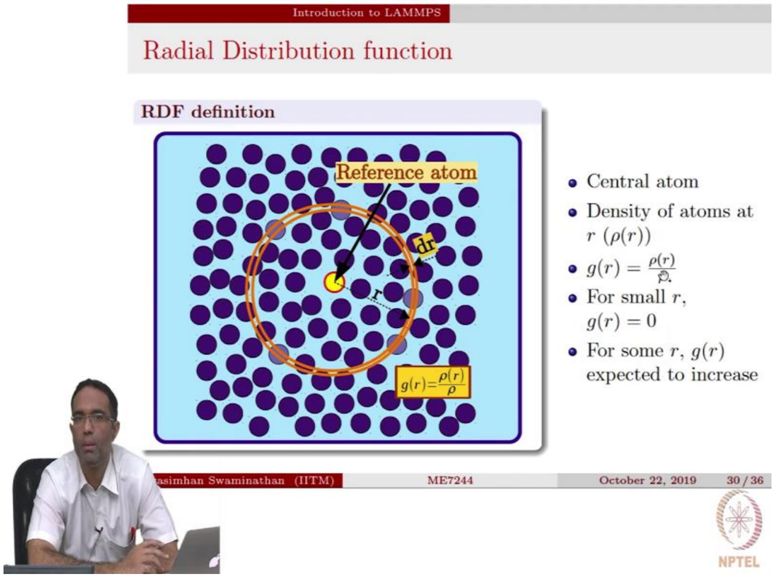

Introduction to LAMMPS

Radial Distribution function

RDF definition

- Central atom
- Density of atoms at r ($\rho(r)$)
- $g(r) = \frac{\rho(r)}{\rho}$
- For small r, $g(r) = 0$
- For some r, $g(r)$ expected to increase

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So, what is the radial distribution function and how it is defined. So the radial distribution function or the pair correlation function g of r, as they will call it, is basically the ratio of the density of atoms at a given distance r from an atom divided by the average density of the sample. So basically number of density, number of atoms per unit volume. So, how this is calculated is, you sit on particular atom and draw a spherical shell, say of thickness dr, at a distance r. And then you basically compute the total number of atoms that are there in that spherical shell divided by the volume of that spherical shell, that would be the density, number density of atoms in that spherical shell. And then divided by n over v which is basically the number density of the entire simulation box that you are looking at.

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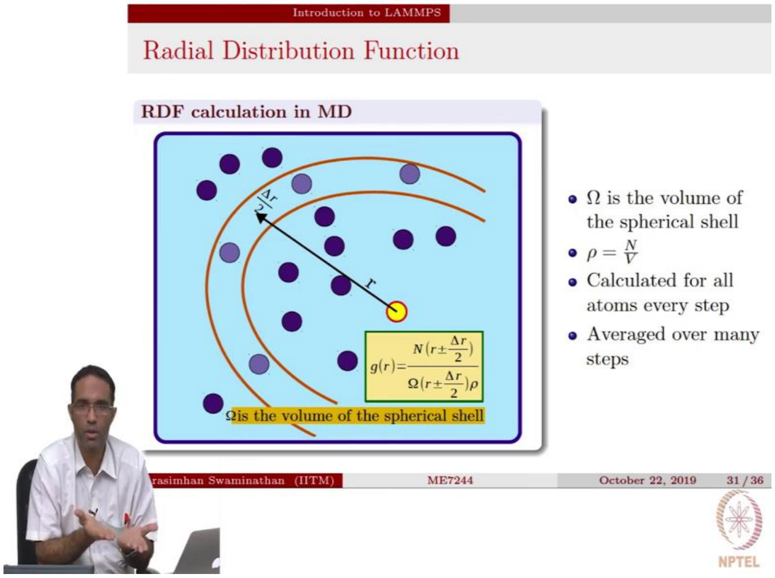

Introduction to LAMMPS

Radial Distribution Function

RDF calculation in MD

$$g(r)=\frac{N\left(r\pm\frac{\Delta r}{2}\right)}{\Omega\left(r\pm\frac{\Delta r}{2}\right)\rho}$$

Ωis the volume of the spherical shell

- Ω is the volume of the spherical shell
- $\rho = \frac{N}{V}$
- Calculated for all atoms every step
- Averaged over many steps

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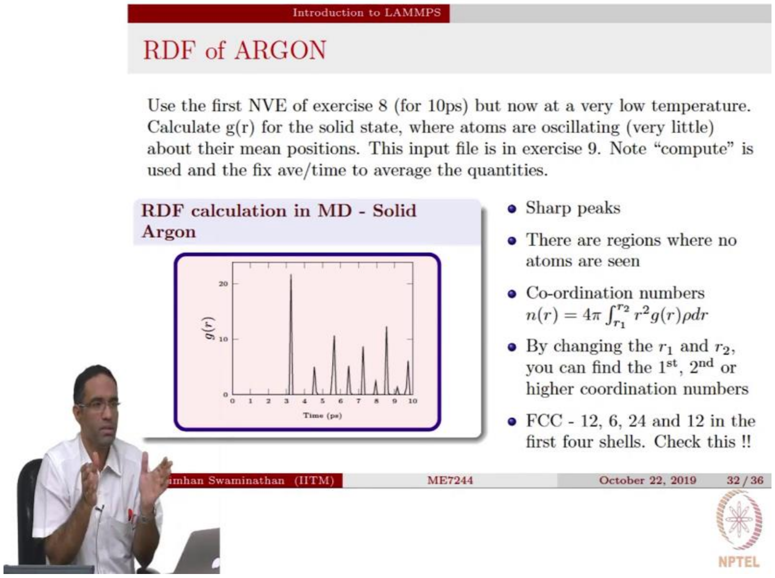
NPTEL



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NPTEL

So, you sit on an atom, this is actually the spherical shell. So, if you look at this spherical shell, you can count how many atoms are basically present so 1,2,3,4 in this case, and then you can divide that by the volume of the shell and then you can divide that entire quantity by the density of the atom. So, this is the expression for g of r that is generally used in molecular dynamics to actually calculate the radial distribution function. So, N is basically the number of atoms in the spherical shell of with delta r and omega is basically the volume of the spherical shell. So, N over omega will be the density at this r and that is being divided by the average density of the system.

And that kind of gives you a measure of what is the probability of finding an atom from a given distance, finding an atom from a given distance in a given distance from the atom that you are sitting. Now, you want to not do this just for one atom in your entire sample, what you want to do is, you want to do this for every atom for some distances and do this for all the atoms and average it, average it over all the atoms and average it over time as well, because all these things could be changing with time since the atoms are oscillating about their mean positions.

So, there are two averages one is you do this for every single atom and then average is the over time, is that, is that clear? So, this quantity g of r is going to be a Vectorial quantity, where for every distance r you have a particular value of g of r. So, that is the reason why it looks, why it has this form where you have large, where you have a peak at a specific distance r. So, this is called the radial distribution function and we have to have two averages, one is over all the atoms and other one is over time. So, this is this should be it should be clear that this actually is for the entire system.

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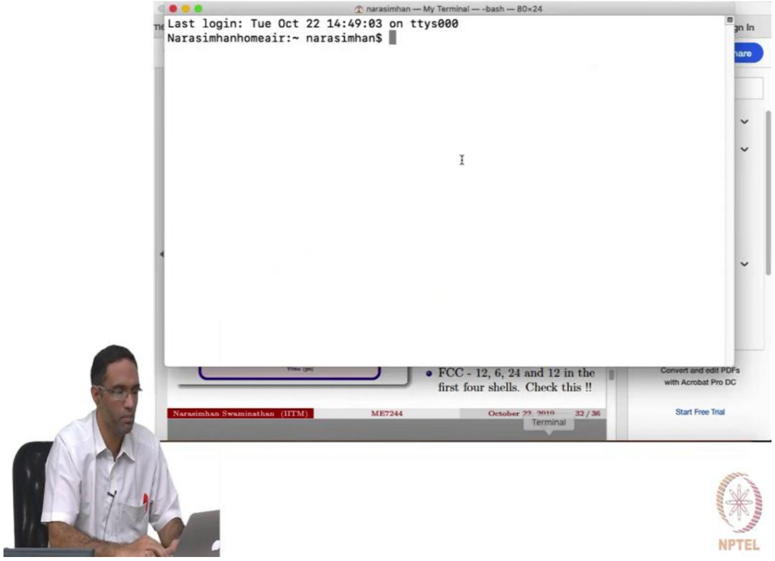

```
Last login: Tue Oct 22 14:49:03 on ttys000
Narasimhanhomeair:~ narasimhan$ 
```

- FCC - 12, 6, 24 and 12 in the first four shells. Check this !!

So, you have to use this fix called fixed average per time in order to…

Student: So, why is it a vector quantity?

Professor: Why it is the vector quantity? So vector quantity because what you are going to get out of this calculation is the following, you are going to get a distance r. And for that distance you are going to get the corresponding g of r. So for various distances, you are going to get various g of r quantities. So what is calculate is actually a vector.

Student: No, had different points in space it had got different values but why should itself, why should that come to itself for direction?

Professor: It is not direction. It is not like a direction, I am not I am just telling you that it is not a scalar. When it is calculated, it is going to be a Vectorial quantity where you have a g of r for every r, that is it. I am not telling you that it is a, it is a vector with direction and all that. I am saying it is a column vector. It is a column. That is why I said it is not like a pressure it is but a column vector, that is what I meant.

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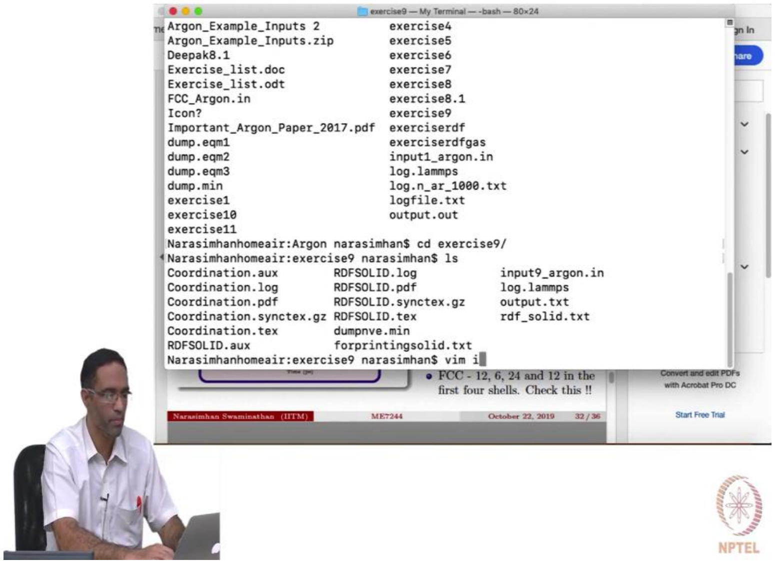
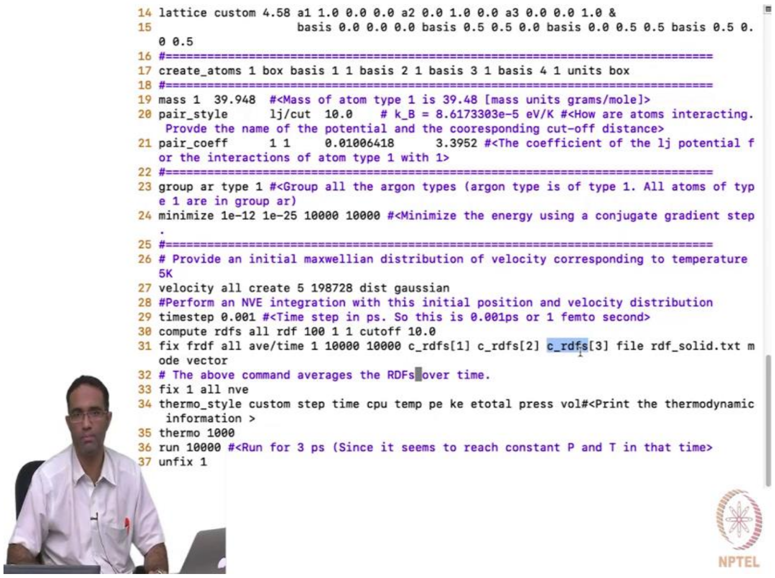
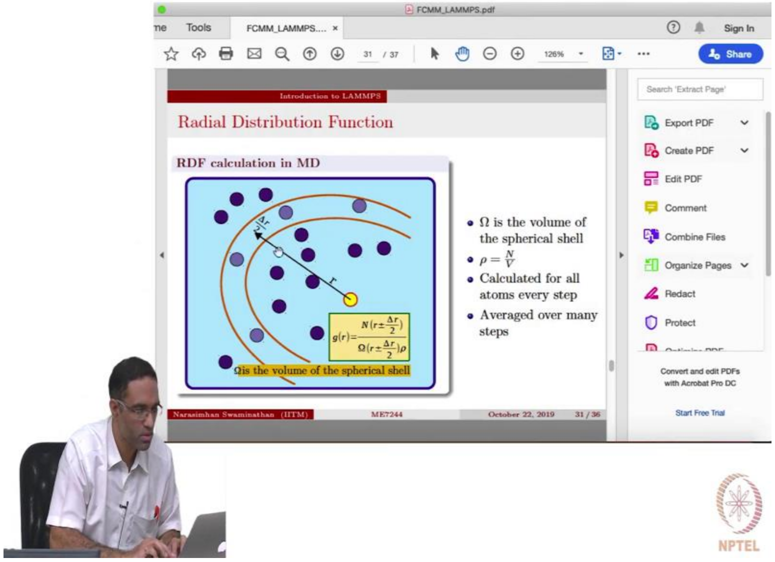


```
Argon_Example_Inputs 2          exercise4
Argon_Example_Inputs.zip        exercise5
Deepak8.1                       exercise6
Exercise_list.doc               exercise7
Exercise_list.odt               exercise8
FCC_Argon.in                    exercise8.1
Icon?                           exercise9
Important_Argon_Paper_2017.pdf  exerciserdf
dump.eqm1                       exerciserdfgas
dump.eqm2                       input1_argon.in
dump.eqm3                       log.lammps
dump.min                        log.n_ar_1000.txt
exercise1                       logfile.txt
exercise10                      output.out
exercise11
Narasimhanhomeair:Argon narasimhan$ cd exercise9/
Narasimhanhomeair:exercise9 narasimhan$ ls
Coordination.aux        RDFSOLID.log            input9_argon.in
Coordination.log        RDFSOLID.pdf            log.lammps
Coordination.pdf        RDFSOLID.synctex.gz     output.txt
Coordination.synctex.gz RDFSOLID.tex            rdf_solid.txt
Coordination.tex        dumpnve.min
RDFSOLID.aux            forprintingsolid.txt
Narasimhanhomeair:exercise9 narasimhan$ vim i
```

- FCC - 12, 6, 24 and 12 in the first four shells. Check this !!



```
lattice custom 4.58 a1 1.0 0.0 0.0 a2 0.0 1.0 0.0 a3 0.0 0.0 1.0 &
                    basis 0.0 0.0 0.0 basis 0.5 0.5 0.0 basis 0.0 0.5 0.5 basis 0.5 0.0 0.5
#=================================================================================
create_atoms 1 box basis 1 1 basis 2 1 basis 3 1 basis 4 1 units box
#=================================================================================
mass 1  39.948  #<Mass of atom type 1 is 39.48 [mass units grams/mole]>
pair_style      lj/cut  10.0    # k_B = 8.6173303e-5 eV/K #<How are atoms interacting. Provde 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 ar)
minimize 1e-12 1e-25 10000 10000 #<Minimize the energy using a conjugate gradient step.
#=================================================================================
# Provide an initial maxwellian distribution of velocity corresponding to temperature 5K
velocity all create 5 198728 dist gaussian
#Perform an NVE integration with this initial position and velocity distribution
timestep 0.001 #<Time step in ps. So this is 0.001ps or 1 femto second>
compute rdfs all rdf 100 1 1 cutoff 10.0
fix frdf all ave/time 1 10000 10000 c_rdfs[1] c_rdfs[2] c_rdfs[3] file rdf_solid.txt mode vector
# The above command averages the RDFs over time.
fix 1 all nve
thermo_style custom step time cpu temp pe ke etotal press vol#<Print the thermodynamic information >
thermo 1000
run 10000 #<Run for 3 ps (Since it seems to reach constant P and T in that time>
unfix 1
```



Radial Distribution Function

RDF calculation in MD

$$g(r)=\frac{N(r\pm\frac{\Delta r}{2})}{\Omega(r\pm\frac{\Delta r}{2})\rho}$$

Ωis the volume of the spherical shell

- Ω is the volume of the spherical shell
- $\rho=\frac{N}{V}$
- Calculated for all atoms every step
- Averaged over many steps

So first let us do this for a solid, I have taken input 9, scholars input 9 is the input file for this, this has already been uploaded on module, so you should be able to find it. So I want to first look at it for a solid. So since I am still working with argon, I better look at extremely low temperatures in order to calculate this radial distribution function. So everything is pretty much the same until we come to this point where I am going to say that you create the last two distributions of about 5 Kelvin, just, just arbitrarily I chose that, and then and I am going to be running NVE simulation and it is during that simulation, I want to gather this data of g of r.

So it is this during this portion that I would be gathering the data for g of r. So this entire thing is just a NVE simulation, which is going to run for about 10000 time steps. Now, over here, I have the command which computes the radial distribution function. So it is again a compute, there are various different compute that we, various computes that we saw in the last class, I showed you a big list in the LAMMPS documentation. And RDF is actually the compute ID, which I am going to refer to later on in the script. All is basically the group of atoms over which I want to make this computation. And this is actually this type, what is a compute style, so it is RDF radial distribution function.

100 is basically the total number of bins between the, the atom that I am sitting at and the maximum radius that I want to examine from the current atom, from every atom. So basically it is, so this would be a cut off distance basically a radius that I am defining and the maximum radius that I can go and then the bins would be the total, the, basically telling me how many such shells that I basically want to take when I am calculating the radial distribution function. So, again, in LAMMPS, this cut off that you give here, get should be equal to or less than the cut off that you give for the potential.

If you want to exanimate more than that, through LAMMPS, you should actually change this value right here or there is some property called, there are some other way by which LAMMPS allows you, allows you to modify the cutoff you should use that. But for this for the purposes of this class 10 angstroms is more than sufficient to examine the radial distribution function. So we will give a cutoff of r and then this is just computing the RDF for one state, we want it to be able to average this quantity for over all the atoms, and then average it over time. So that is basically done by this command right here, where you say fix.

Again, this is a fix ID, all the atoms averaged over time but now it is not average per atoms, average over time of this global quantity, and this should now be clear to you, I am running for 10000 steps. So I want to run I want to print out every 10000 steps, which means I want to have only 1 average over the entire run. This is basically the number of steps that I want to choose which is also 10000 and 1 is basically the every take every step, take input from every step that you compute the RDF and then the compute basically prints out is capable is actually a an array. So, you have C underscore RDF of 1 which will basically contain the values of the corresponding r’s C RDF of 2 will basically contain the corresponding g of r’s and C underscore rdfs of 3 is going to contain the corresponding integral which is basically the which is related to the coordination number of the of the atom at that spot.

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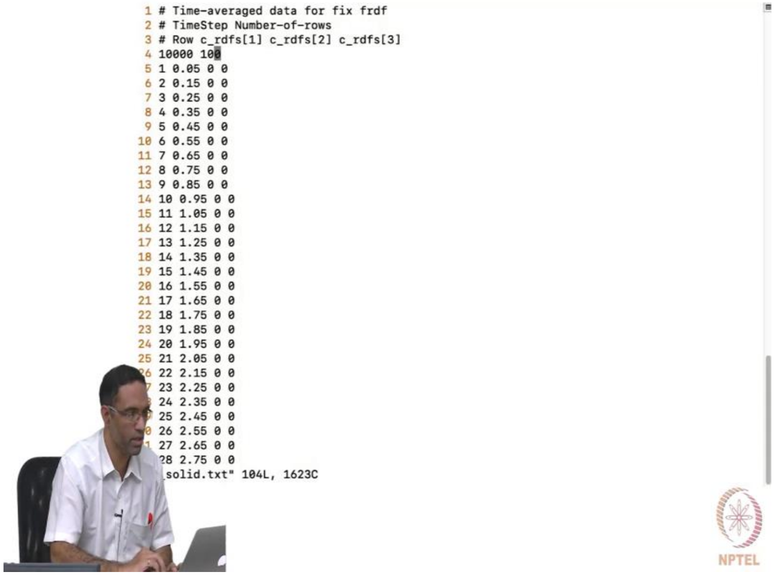
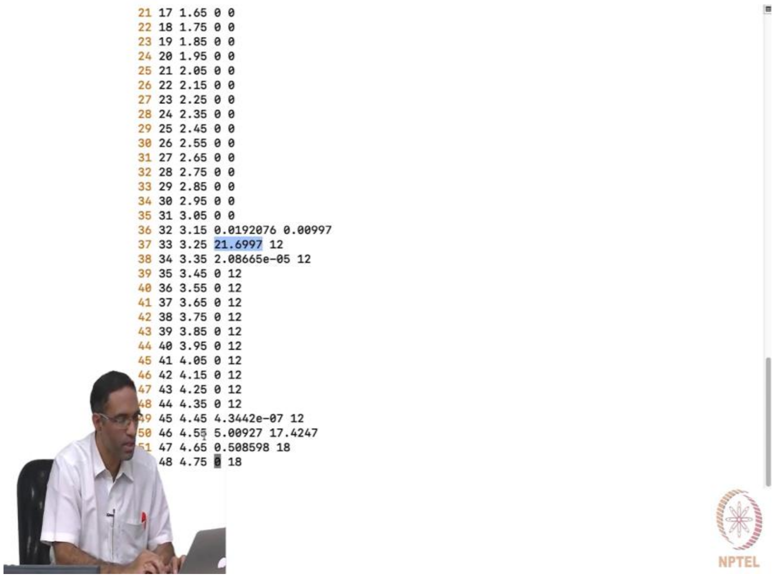
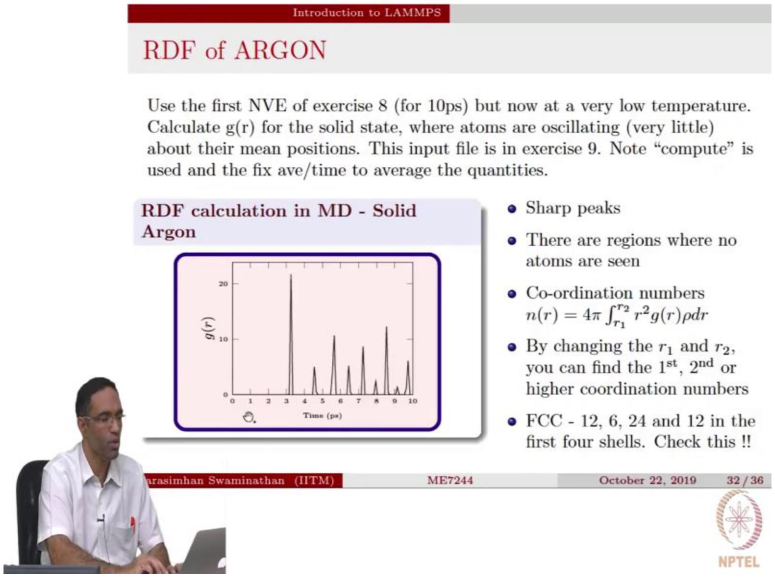
```
Makefile                          eclipse-workspace
Narasimhanhomeair:~ narasimhan$ cd Dropbox/MAterials_Course/Molecular_Dynamic/Argon/
Narasimhanhomeair:Argon narasimhan$ s
-bash: s: command not found
Narasimhanhomeair:Argon narasimhan$ ls
Ar_1000_Kr_0.txt                  exercise2
Argon_Example_Inputs              exercise3
Argon_Example_Inputs 2            exercise4
Argon_Example_Inputs.zip          exercise5
Deepak8.1                         exercise6
Exercise_list.doc                 exercise7
Exercise_list.odt                 exercise8
FCC_Argon.in                      exercise8.1
Icon?                             exercise9
Important_Argon_Paper_2017.pdf    exerciserdf
dump.eqm1                         exerciserdfgas
dump.eqm2                         input1_argon.in
dump.eqm3                         log.lammps
dump.min                          log.n_ar_1000.txt
exercise1                         logfile.txt
exercise10                        output.out
exercise11
Narasimhanhomeair:Argon narasimhan$ cd exercise9/
Narasimhanhomeair:exercise9 narasimhan$ ls
Coordination.aux        RDFSOLID.log            input9_argon.in
 oordination.log        RDFSOLID.pdf            log.lammps
 ordination.pdf         RDFSOLID.synctex.gz     output.txt
 ordination.synctex.gz RDFSOLID.tex            rdf_solid.txt
 ordination.tex         dumpnve.min
 FSOLID.aux             forprintingsolid.txt
  asimhanhomeair:exercise9 narasimhan$ vim input9_argon.in
   imhanhomeair:exercise9 narasimhan$ vim input9_argon.in
    mhanhomeair:exercise9 narasimhan$ vim rdf_solid.txt
```



```
# Time-averaged data for fix frdf
# TimeStep Number-of-rows
# Row c_rdfs[1] c_rdfs[2] c_rdfs[3]
10000 100
1 0.05 0 0
2 0.15 0 0
3 0.25 0 0
4 0.35 0 0
5 0.45 0 0
6 0.55 0 0
7 0.65 0 0
8 0.75 0 0
9 0.85 0 0
10 0.95 0 0
11 1.05 0 0
12 1.15 0 0
13 1.25 0 0
14 1.35 0 0
15 1.45 0 0
16 1.55 0 0
17 1.65 0 0
18 1.75 0 0
19 1.85 0 0
20 1.95 0 0
21 2.05 0 0
22 2.15 0 0
23 2.25 0 0
24 2.35 0 0
25 2.45 0 0
26 2.55 0 0
27 2.65 0 0
28 2.75 0 0
solid.txt" 104L, 1623C
```



```
17 1.65 0 0
18 1.75 0 0
19 1.85 0 0
20 1.95 0 0
21 2.05 0 0
22 2.15 0 0
23 2.25 0 0
24 2.35 0 0
25 2.45 0 0
26 2.55 0 0
27 2.65 0 0
28 2.75 0 0
29 2.85 0 0
30 2.95 0 0
31 3.05 0 0
32 3.15 0.0192076 0.00997
33 3.25 21.6997 12
34 3.35 2.08665e-05 12
35 3.45 0 12
36 3.55 0 12
37 3.65 0 12
38 3.75 0 12
39 3.85 0 12
40 3.95 0 12
41 4.05 0 12
42 4.15 0 12
43 4.25 0 12
44 4.35 0 12
45 4.45 4.3442e-07 12
46 4.55 5.00927 17.4247
47 4.65 0.508598 18
48 4.75 0 18
```



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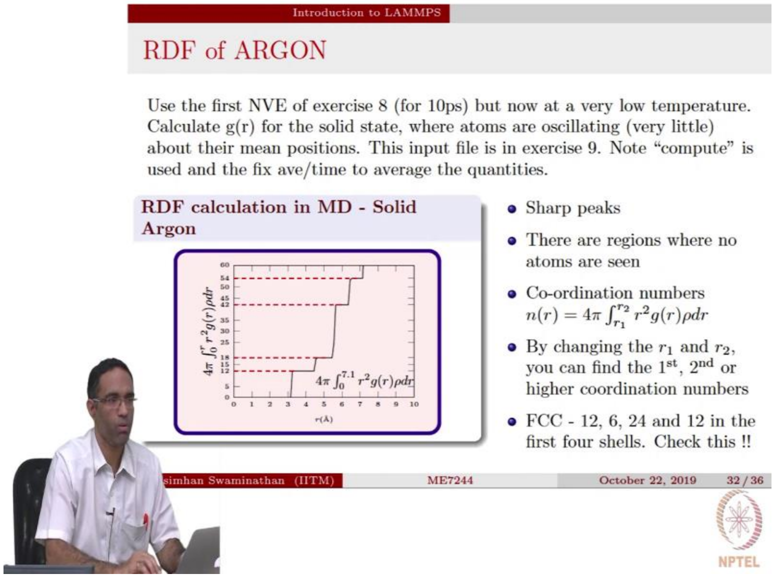

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So, the fixed rdf, if you, so what did I use? What file name would I use? I use RDF underscore solid dot txt. So, vim rdf underscore solid dot txt it looks like this. So, it has some time average data for fix rdf, time step, number of rows. This is the time step 10000, that is, that is what we want averaged over all the 10000 times step, number of rows is 100. And this is basically the no sorry, this is not the, this is the, it prints four things, prints four things. The first is just a serial number. The second one is basically the corresponding value of r. The third column is the corresponding g of r for that data and the third one is the integral of g of r. The integral of g of r, what does it give you? It gives you basically the coordination of that point, exactly.

So, I will just show it show that to you in the next. So, this is this is what this code has generated. So, as you can see, initially it is all look at this, this third column here, it is all 0 initially, and then it starts to raise, it starts to raise to some large value 21.6997 and then again, it starts to decrease to 0. And again, it raises to some value and keeps going on and on. So, this is how the RDF of the solid looks like and this is the plot that it basically generates. So, you know that the first. So, what is the what is the distance? So, the what was, there is some lattice constant that we have used, I think we have used 4.58.

So, what is the first neighbor in the FCC, this FCC lattice also, what is the first neighbor in the FCC lattice?

Student: a by root 2.

Professor: a by root 2. So, you can plug it in here and see if the first peak basically occurs approximately at that point.

Student: First neighbor…

Professor: Any atom you sit on any atom and keep going, the first atom that you encounter, the first atom that you encounter will be at a distance of a by root 2. That is this number right here. So, this is actually a signature of whether it is BCC or FCC. You can actually calculate the lattice constant by looking at this. If you knew the structure is BCC, then you can actually calculate the lattice constant by looking at this diagram because this is the first neighbor respond here, second neighbor respond here, third neighbors respond here fourth neighbor respond here and so on.

And then the integral of g of r, actually, it is the integral over the sphere. Because you are integrating, because you are always considered a sphere in this particular case. So, 4 phi integral from r1 to r2 r square g of r is going to give you the total number of atoms that is present at that particular distance between r1 and r2. So, by changing r1 and r2, we can find the first, second, third and fourth so on nearest neighbors, that is actually appropriate for this particular material model for this particular material. And for FCC, the first nearest, number of first nearest neighbors is 12, then is 6, the next, next distance you will find only 6 neighbors. After that you find actually 24 neighbors, after that you find 12 neighbors.

Of course, we would not have thought about such far of distances, which is precisely the reason why you can actually use this information to get that. So this is just plotting the final column of the radial distribution function, which is that the integral from 0 to 1, 0 to 2, 0 to 3,0 to 4 is what is being plotted here. So, as you can see at the point where you are the first nearest neighbor, you will get 12. So, it is first nearest neighbor, number of first nearest neighbor for every atom is 12.

The next is 18, which is basically 12 plus the 6 nearest neighbors because this involves an integral from 0 to the second nearest neighbor distance. Then you have from 12 to 42, which is basically plus 24. So, 12 plus 16 plus 24 and so on. So, this will tell you the, this is kind of indicating to you what is the number of number of first nearest neighbors, second nearest neighbors present with the crystal structure. So, this sort of information can be obtained by looking at the radial distribution function and the calculation… Yes?

Student: In the graph of g of r versus r it is again averaged with all the r's also I mean all the atoms.

Professor: All the atoms.

Student: So how do we associate meaning to get r?

Professor: Which r?

Student: Like where is our reference point?

Professor: At every atom, sit on every atom. Sit on every atom draw radius of 10 angstroms divide into 100 bins, start looking at how many atoms are there, sum it all, keep that in an array, sit on another atom, do this, add them up, sit on another atom, do this add them up. Keep doing it over and over again until you are done with all the atoms by keeping in mind the periodic boundary conditions because an atom, an atom at the end is actually closer to the atom on the other end, it is not far away, because it is actually located here. So keeping in mind, the periodic image of every atom, you should do this for all the atoms, you can take some time to write such a code, because that is why LAMMPS actually does this for you and it is pretty useful.

Student: Sir is it the reference each time?

Professor: Yes, it sits on each atom each time.

Student: So basically what is being done is that for each atom RDF is being calculated, then it is being some average for the entire system?

Professor: And average over time also, because if the atoms are actually… Yeah, because for this case, it might not have made a huge difference, because the atoms are hardly oscillating, but say you want to obtain the radial distribution function at some finite temperature like 300 Kelvin or 400 Kelvin, then the atoms are actually oscillating about their mean positions. So one, at one specific, at every single short, the atoms are not exactly in the FCC positions, there may be minor deviations because they are oscillating, is not it?

So if you really want to see the FCC structure, you have to average them out over time as well, so that you can, in fact, see that it is still a solid, the atoms are just vibrating about their mean positions.

Student: would there be seen as calculating an average function and then doing the average?

Professor: Yes, yes, it should be the same. Yup.

Student: Sir if we want to use this…

Professor: But that would be very hard to do, every time you have to generate. So this one has generated 10000 different configuration. Now, you are, if what, what you are saying is generate (additional), generate 10000 different random positions for each atom and then average it out. Yeah, this is the same thing.

Student: Even one thing with this formula for calculating the…

Professor: This one, 4 pi. Yes.

Student: Calculating nr at distance of…

Professor: Between r1 and r2, total number of atoms that you can find from a given atom between the distance r1 and r2, from r1 to r2 how many atoms are there surrounding any given atom.

Student: So, there should be a difference between upper limit and lower limit, no matter how small that is?

Professor: Yes, yes.

Student: But if you want a specific distance you can make that difference very, very small.

Professor: You will get 0 if there is no atom. Yeah, if there is no atom you will get 0. Any, anything specific?

Student: Sir this question was regarding change of order of integration?

Professor: Whose question?

Student: first we average over all the coordinates of space and then….

Professor: No what he says is instead of averaging it over a time you have different ensembles, this is, instead of saying time average, he says do ensemble average. You have different positions of each and then do the same thing, it is a same thing because time averaging and phase averaging or same or ensemble average is the same.

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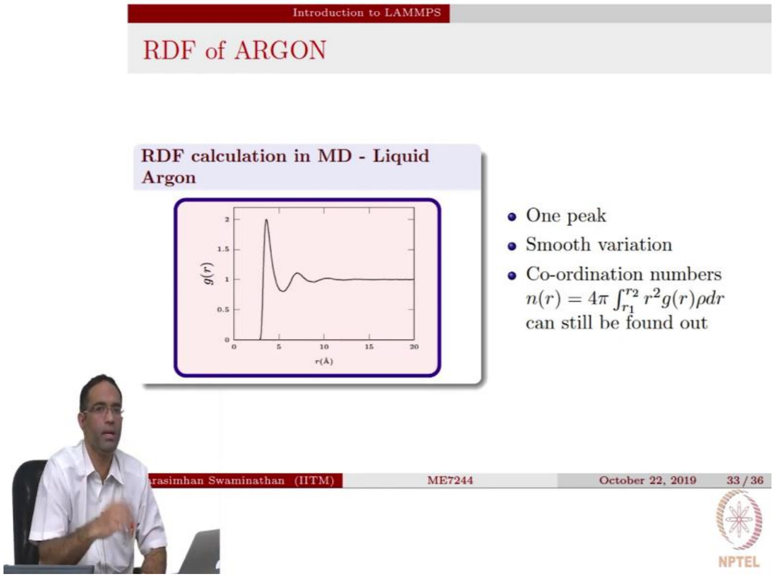


Introduction to LAMMPS

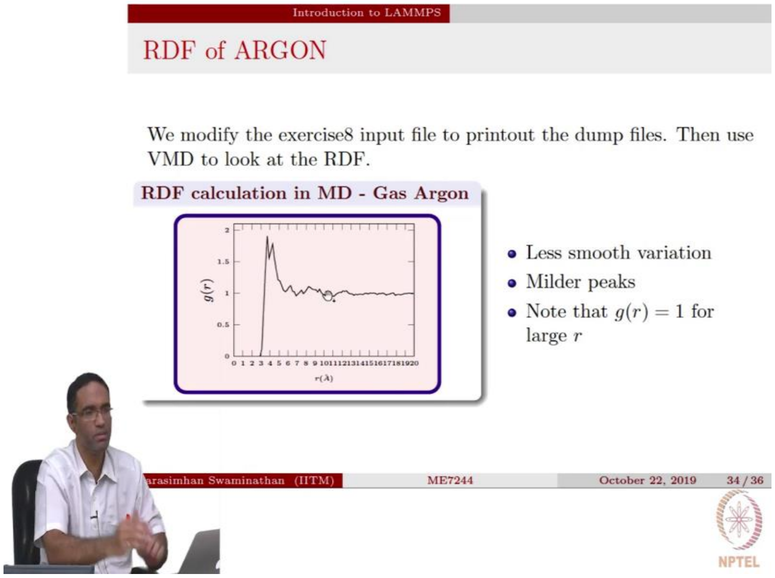
RDF of ARGON

RDF calculation in MD - Liquid Argon

- One peak
- Smooth variation
- Co-ordination numbers $n(r) = 4\pi \int_{r_1}^{r_2} r^2 g(r) \rho dr$ can still be found out

So, this is how it looks for liquid, there is one single peak showing some sort of short range order, but after that you find one small peak and then the radial distribution function converges to 1 basically telling you that the probability of you finding an atom from if you sit on any atom, if you go far enough, there is always a probability, the probability of finding another atom is 1. That is what this is basically telling you., this is how it looks for liquid.

(Refer Slide Time: 20:51)



Introduction to LAMMPS

RDF of ARGON

We modify the exercise8 input file to printout the dump files. Then use VMD to look at the RDF.

RDF calculation in MD - Gas Argon

- Less smooth variation
- Milder peaks
- Note that $g(r) = 1$ for large r

And this is something that, it looks for solid you do not see this additional peak. So, even shorter range order is found for gases.

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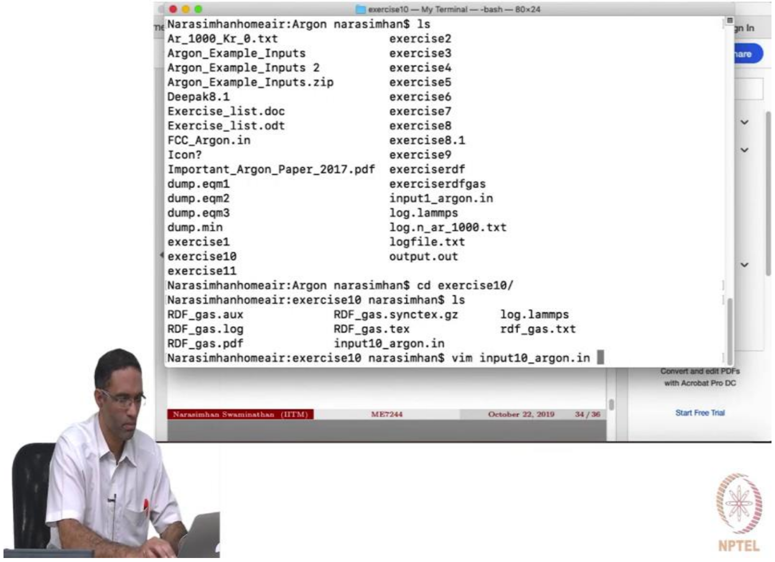
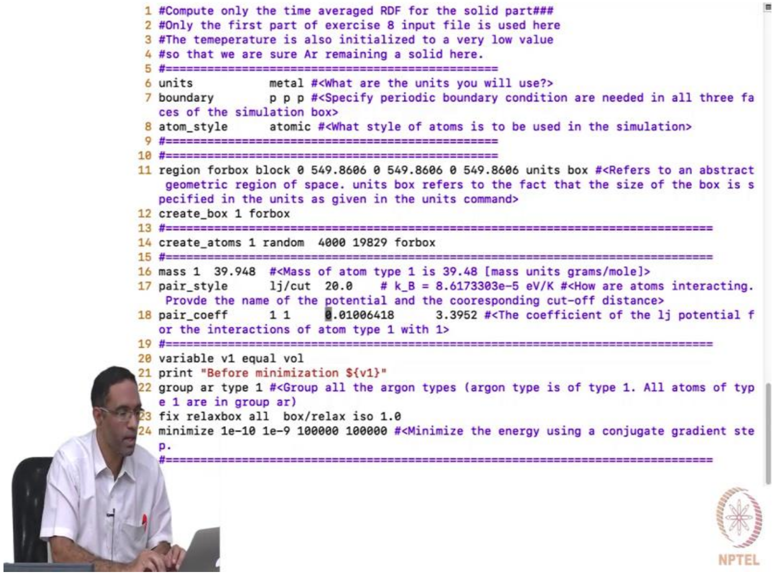
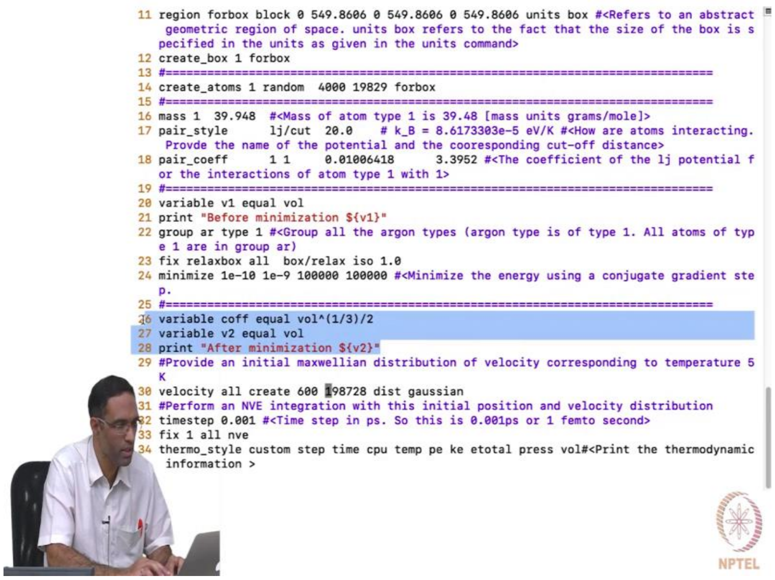


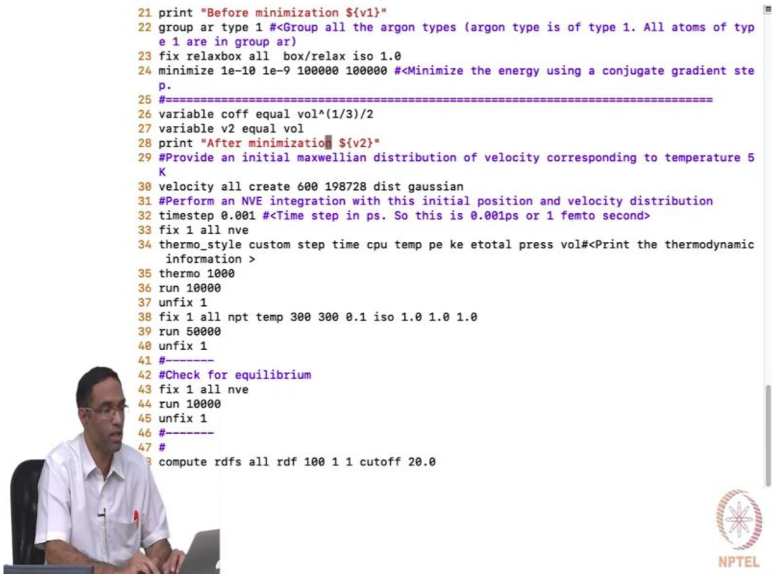
```
Narasimhanhomeair:Argon narasimhan$ ls
Ar_1000_Kr_0.txt                exercise2
Argon_Example_Inputs            exercise3
Argon_Example_Inputs 2          exercise4
Argon_Example_Inputs.zip        exercise5
Deepak8.1                       exercise6
Exercise_list.doc               exercise7
Exercise_list.odt               exercise8
FCC_Argon.in                    exercise8.1
Icon?                           exercise9
Important_Argon_Paper_2017.pdf  exerciserdf
dump.eqm1                       exerciserdfgas
dump.eqm2                       input1_argon.in
dump.eqm3                       log.lammps
dump.min                        log.n_ar_1000.txt
exercise1                       logfile.txt
exercise10                      output.out
exercise11
Narasimhanhomeair:Argon narasimhan$ cd exercise10/
Narasimhanhomeair:exercise10 narasimhan$ ls
RDF_gas.aux             RDF_gas.synctex.gz      log.lammps
RDF_gas.log             RDF_gas.tex             rdf_gas.txt
RDF_gas.pdf             input10_argon.in
Narasimhanhomeair:exercise10 narasimhan$ vim input10_argon.in
```



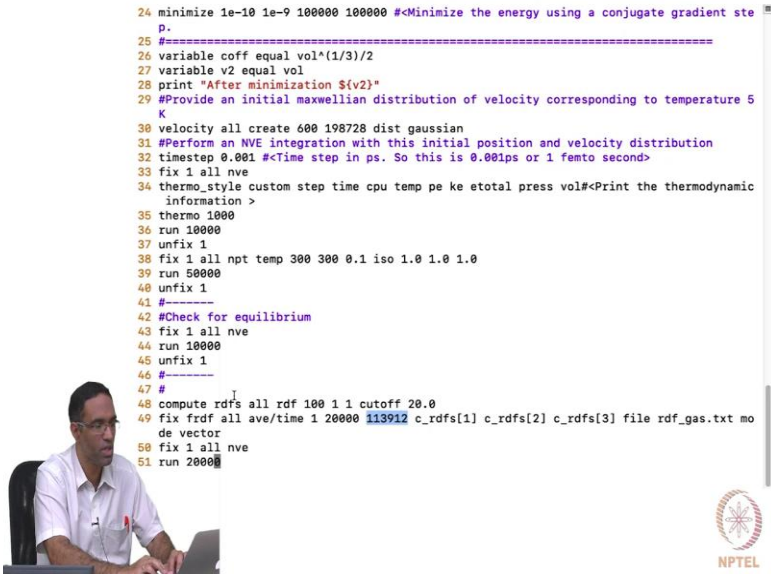
```
#Compute only the time averaged RDF for the solid part###
#Only the first part of exercise 8 input file is used here
#The temeperature is also initialized to a very low value
#so that we are sure Ar remaining a solid here.
#==============================================
units           metal #<What are the units you will use?>
boundary        p p p #<Specify periodic boundary condition are needed in all three fa
ces of the simulation box>
atom_style      atomic #<What style of atoms is to be used in the simulation>
#==============================================
#==============================================
region forbox block 0 549.8606 0 549.8606 0 549.8606 units box #<Refers to an abstract
 geometric region of space. units box refers to the fact that the size of the box is s
pecified in the units as given in the units command>
create_box 1 forbox
#============================================================================
create_atoms 1 random  4000 19829 forbox
#============================================================================
mass 1  39.948  #<Mass of atom type 1 is 39.48 [mass units grams/mole]>
pair_style      lj/cut  20.0    # k_B = 8.6173303e-5 eV/K #<How are atoms interacting.
 Provde 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 f
or the interactions of atom type 1 with 1>
#============================================================================
variable v1 equal vol
print "Before minimization ${v1}"
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)
fix relaxbox all  box/relax iso 1.0
minimize 1e-10 1e-9 100000 100000 #<Minimize the energy using a conjugate gradient ste
p.
#============================================================================
```



```
region forbox block 0 549.8606 0 549.8606 0 549.8606 units box #<Refers to an abstract geometric region of space. units box refers to the fact that the size of the box is specified in the units as given in the units command>
create_box 1 forbox
#===========================================================================
create_atoms 1 random  4000 19829 forbox
#===========================================================================
mass 1  39.948  #<Mass of atom type 1 is 39.48 [mass units grams/mole]>
pair_style      lj/cut  20.0    # k_B = 8.6173303e-5 eV/K #<How are atoms interacting. Provde 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>
#===========================================================================
variable v1 equal vol
print "Before minimization ${v1}"
group ar type 1 #<Group all the argon types (argon type is of type 1. All atoms of type 1 are in group ar)
fix relaxbox all  box/relax iso 1.0
minimize 1e-10 1e-9 100000 100000 #<Minimize the energy using a conjugate gradient step.
#===========================================================================
variable coff equal vol^(1/3)/2
variable v2 equal vol
print "After minimization ${v2}"
#Provide an initial maxwellian distribution of velocity corresponding to temperature 5 K
velocity all create 600 198728 dist gaussian
#Perform an NVE integration with this initial position and velocity distribution
timestep 0.001 #<Time step in ps. So this is 0.001ps or 1 femto second>
fix 1 all nve
thermo_style custom step time cpu temp pe ke etotal press vol#<Print the thermodynamic information >
```



```
print "Before minimization ${v1}"
group ar type 1 #<Group all the argon types (argon type is of type 1. All atoms of type 1 are in group ar)
fix relaxbox all  box/relax iso 1.0
minimize 1e-10 1e-9 100000 100000 #<Minimize the energy using a conjugate gradient step.
#===========================================================================
variable coff equal vol^(1/3)/2
variable v2 equal vol
print "After minimization ${v2}"
#Provide an initial maxwellian distribution of velocity corresponding to temperature 5 K
velocity all create 600 198728 dist gaussian
#Perform an NVE integration with this initial position and velocity distribution
timestep 0.001 #<Time step in ps. So this is 0.001ps or 1 femto second>
fix 1 all nve
thermo_style custom step time cpu temp pe ke etotal press vol#<Print the thermodynamic information >
thermo 1000
run 10000
unfix 1
fix 1 all npt temp 300 300 0.1 iso 1.0 1.0 1.0
run 50000
unfix 1
#-------
#Check for equilibrium
fix 1 all nve
run 10000
unfix 1
#-------
#
compute rdfs all rdf 100 1 1 cutoff 20.0
```



```
minimize 1e-10 1e-9 100000 100000 #<Minimize the energy using a conjugate gradient step.
#============================================================================
variable coff equal vol^(1/3)/2
variable v2 equal vol
print "After minimization ${v2}"
#Provide an initial maxwellian distribution of velocity corresponding to temperature 5K
velocity all create 600 198728 dist gaussian
#Perform an NVE integration with this initial position and velocity distribution
timestep 0.001 #<Time step in ps. So this is 0.001ps or 1 femto second>
fix 1 all nve
thermo_style custom step time cpu temp pe ke etotal press vol#<Print the thermodynamic information >
thermo 1000
run 10000
unfix 1
fix 1 all npt temp 300 300 0.1 iso 1.0 1.0 1.0
run 50000
unfix 1
#-------
#Check for equilibrium
fix 1 all nve
run 10000
unfix 1
#-------
#
compute rdfs all rdf 100 1 1 cutoff 20.0
fix frdf all ave/time 1 20000 113912 c_rdfs[1] c_rdfs[2] c_rdfs[3] file rdf_gas.txt mode vector
fix 1 all nve
run 20000
```

So, the gas code is also here. So it is, so, I generated this input file for the gas slightly differently. So, what I have done is I have used my previous experience on what the volume should be for 1 atmosphere and 300 Kelvin from exercise 8 I really know the volume. So, from there I can actually construct the block size. And after that, see this, there are some new commands here, so, I should specify that So, this gas state, gaseous state was not done like what was done for the for exercise 8. In exercise 8 we were learning several things. So, we started off from really weird configuration and then we slowly equilibrated the system to actually be able to generate a system which was at equilibrium, 1 atmosphere and 300 Kelvin.

Now, I do not want all that, I just want the gas, I want to gas. From previous experience I have figured out that my gas at 300 Kelvin at 1 atmosphere, the system volume is something that turned out to be something and the cube root of that volume is basically giving me my box dimensions, which is what this 549.8606 is. Then what I have done after creating the box, I have to throw in atoms inside the box at random positions because now there is no structure to this whole gas. So, I want to throw 4000 atoms remember the previous case also we had only 4000 atoms 445.8, 45.8, 4.58 generated 10 by 10 by 10 unit cells which had about 4000 atoms.

So you had, so I just say create atoms 1 random, at random positions create 4000 atoms, this is the corresponding random seed and this is basically the region where I want to generate all these atoms. So, it just generates all these atoms. After doing that of course, everything else is the same. I just want to calculate the volume for whatever reason. So, I then after that I have introduced here another command. So, remember previously when we minimized the system, it just minimized holding the box fixed that means the box dimensions are fixed. There is also another command here, where as it is performing the minimization, you may be able to adjust the box sizes, you may not necessarily have to start off the NPT from really far of state from what you require.

So for that you have a fixed call fix relax box all, relax box is basically a fix id it is not a key word of LAMMPS, this is a key word of LAMMPS which is box slash relax isotropic and the corresponding pressure. So, this one can also adjust the size of the box really well. What it does is, as it is performing this minimization, it will perform these minor changes. So, this is a new command that you need to you can learn then I give a high velocity here, all these things, all these things may not be needed for this particular exercise. Basically just creating a very high temperature distribution or a very high temperature and then equilibrating it for long enough. And then I do a NPT for a very, very, for about 50000 steps which may not be needed. I just wanted to make sure that it equilibrated at 300 Kelvin.

We saw previously that 50000 from a really far of state was also sufficient for this case, for this for since I have already given reasonably good starting configuration by using the right volume of the box and also did a fix relax box after that, this NPT may not need so much, but I have just given it here. Then I checked for equilibration and then performed compute of the RDF in exactly the same manner. And again I performed the RDF only in the last final NVE, this is a so 20000. This happens to be the final time step that you will reach until this point, like what we discuss yesterday, this one. So it is going to print out the data, every 113912 time step, and you are going to average over 20000 steps, every steps and the same information is actually printed.

(Refer Slide Time: 26:04)

So, so take a look at it looks something like this and again it kind of converges to the value 1. So this is the way you can use LAMMPS to actually calculate your radial distribution function. Now, a lot of features have come in this visualization software called Ovito, which can also calculate the radial distribution function. So, yeah?

Student: So how to get that 113912 time steps or like…

Professor: But it is easy, you know how many steps you have run. So, it should not be too hard to do that.

Student: But if I…

Professor: Or you can define compute. You can you can define a compute to calculate the total number of time steps, calculate it.

Student: Sir it seems like it is some way we are half coding, now if I do some playing around and I have to keep…

Professor: You have to keep this in mind, you have to keep this in mind or you can make everything a variable, run also can be made a variable then you can keep that and you can add them to variable equal and add them and then give that value here.

Student: Sir what difference between the equilibriums? Now what difference are we looking at?

Professor: What is that? What is the difference you get?

Student: When we use relax box instead of using the previous command…

Professor: NPT. Fixed relax box has a very rough relaxation just approximately changes the dimensions of the box so as to make the system to get as close to the pressure that you want. It is not really a barostat. It is not something that is going to maintain the pressure over time or anything. During the process of minimizing, the energy of the system, it does a little bit of adjusting the box sizes. That is it. After that you still may have to do, mostly you have to do NPT. But if you are starting off from a really far off configuration, this can be a crude way to actually bring the system to approximately the size that you want.

Did you, did you notice when we did the previous exercise 8, when I showed it to you in Ovito, you start off from a really small box, and this thing just became extremely large. Now go and try that by first using a fixed, fixed box relax following that try to do NPT, the minimize structure itself will be quite large. And after that, the NPT will have to do a little bit of adjustment in order to bring the box to the closing, make it more accurate. Basically, NPT is only fine tuning, rather than rapidly changing stuff. These things are important because when you are working with solids, it will play a very important role.

Student: The g of r is a probability?

Professor: Yes.

Student: It is not really a probability?

Professor: Is not?

Student: It is not really a probability because…

Professor: It is not really a (probability), density at r divided by the average density. So it kind of gives you the probability of…

Student: it goes above 1.

Professor: Yes, in that sense, yes. This is not like I said, it is a like it is like a probability. It is a probability that you will find an atom at the distance. If you see a peak, you have, it is a probability that you will find an atom at the distance.

Student: It is like abundance with respect to…

Professor: It is more like?

Student: An abundance.

Professor: Abundance.

Student: Or multiples of the ideal value?

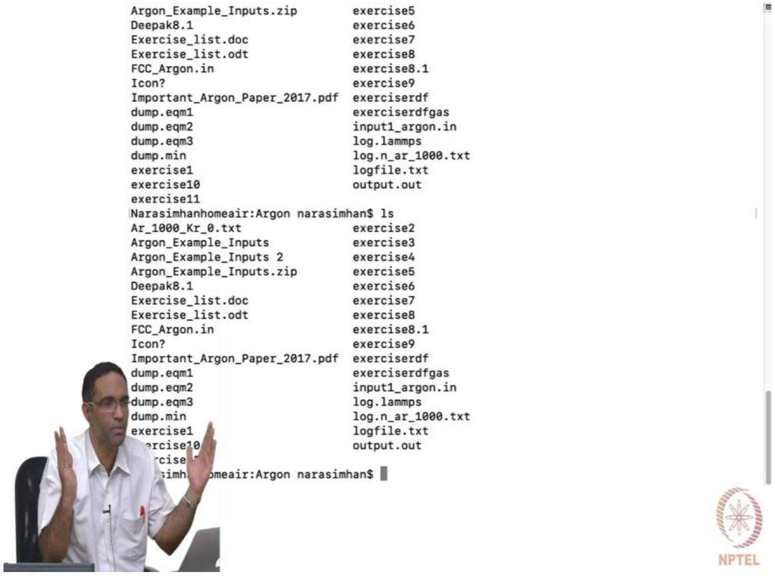
Student: Is it more the number of atoms or is it the higher peak the more the chances of atoms?

Professor: Higher the peak, the more the chances.

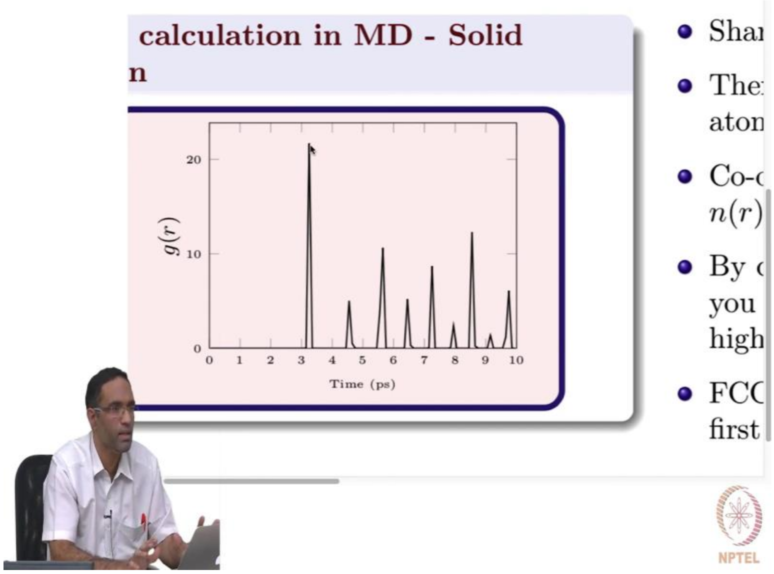
Student: It is a probability but not exactly a probability…

Professor: Correct. Correct. You normalize it to 1.

(Refer Slide Time: 30:06)



```
Argon_Example_Inputs.zip        exercise5
Deepak8.1                       exercise6
Exercise_list.doc               exercise7
Exercise_list.odt               exercise8
FCC_Argon.in                    exercise8.1
Icon?                           exercise9
Important_Argon_Paper_2017.pdf  exerciserdf
dump.eqm1                       exerciserdfgas
dump.eqm2                       input1_argon.in
dump.eqm3                       log.lammps
dump.min                        log.n_ar_1000.txt
exercise1                       logfile.txt
exercise10                      output.out
exercise11
Narasimhanhomeair:Argon narasimhan$ ls
Ar_1000_Kr_0.txt                exercise2
Argon_Example_Inputs            exercise3
Argon_Example_Inputs 2          exercise4
Argon_Example_Inputs.zip        exercise5
Deepak8.1                       exercise6
Exercise_list.doc               exercise7
Exercise_list.odt               exercise8
FCC_Argon.in                    exercise8.1
Icon?                           exercise9
Important_Argon_Paper_2017.pdf  exerciserdf
dump.eqm1                       exerciserdfgas
dump.eqm2                       input1_argon.in
dump.eqm3                       log.lammps
dump.min                        log.n_ar_1000.txt
exercise1                       logfile.txt
  ercise10                      output.out
  rcise
  simh   omeair:Argon narasimhan$ 
```


calculation in MD - Solid
n

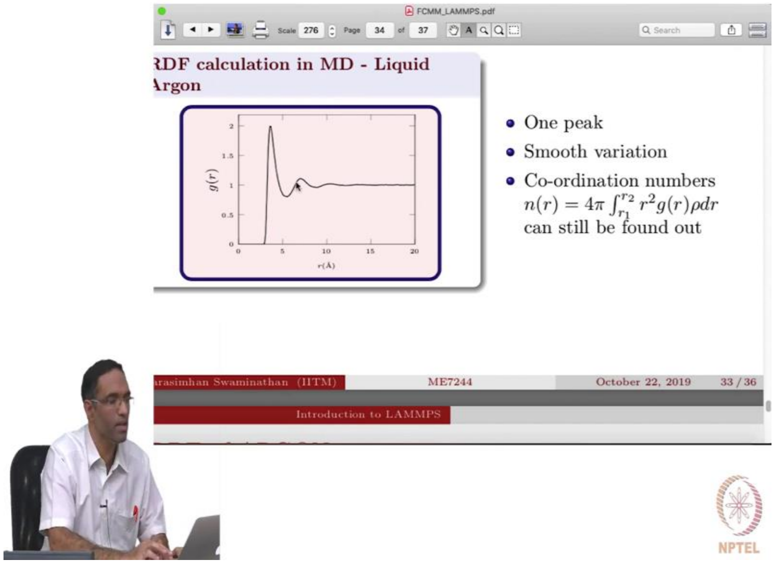
- Shar
- The
aton
- Co-c
$n(r)$
- By c
you
high
- FCC
first

So it is okay, it is okay if it is not exactly viewed as being a probability, per say, but it should not be too hard to accept that. If you look at this figure, so at this point, just there is a peak. So it essentially means that the chances of finding an atom there are high., that is it. So it is very clear that here there is no chance of finding any atom. So in that sense, it is kind of a measure of the probability of finding an atom at this distance from a given atom.

Student: Sir in that case for the fluid and gas, after times in course kind of straight line, so how, how you will explain this?

Professor: What is that, at kind of become straight line, what is the meaning of this? It means that the density of the gas at any distance r and the density of the actual system is the same. So there is always some atom present at a distance.

(Refer Slide Time: 31:07)



RDF calculation in MD - Liquid Argon

- One peak
- Smooth variation
- Co-ordination numbers $n(r) = 4\pi \int_{r_1}^{r_2} r^2 g(r) \rho dr$ can still be found out

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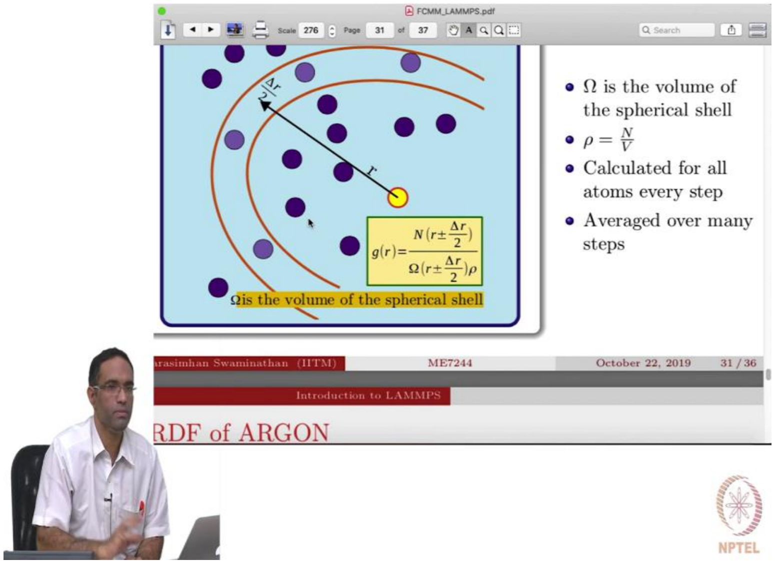
Introduction to LAMMPS

This this peak here shows that there is some sort of a short range order that is being present there are if you are small distances, you always tend to find a little bit more atom, atom such present for every atom. But as you go far away, it kind of reaches the average density of the entire system. That is what it means.

(Refer Slide Time: 31:39)



$$g(r) = \frac{N(r \pm \frac{\Delta r}{2})}{\Omega(r \pm \frac{\Delta r}{2})\rho}$$

Ωis the volume of the spherical shell

- Ω is the volume of the spherical shell
- $\rho = \frac{N}{V}$
- Calculated for all atoms every step
- Averaged over many steps

arasimhan Swaminathan (IITM) ME7244 October 22, 2019 31 / 36

Introduction to LAMMPS

RDF of ARGON

Student: Sir in g of r is equal to rho of r by rho, the formula which we first saw, there the denominator rho represents the…

Professor: N by V, number of atoms divided by the volume of the system.

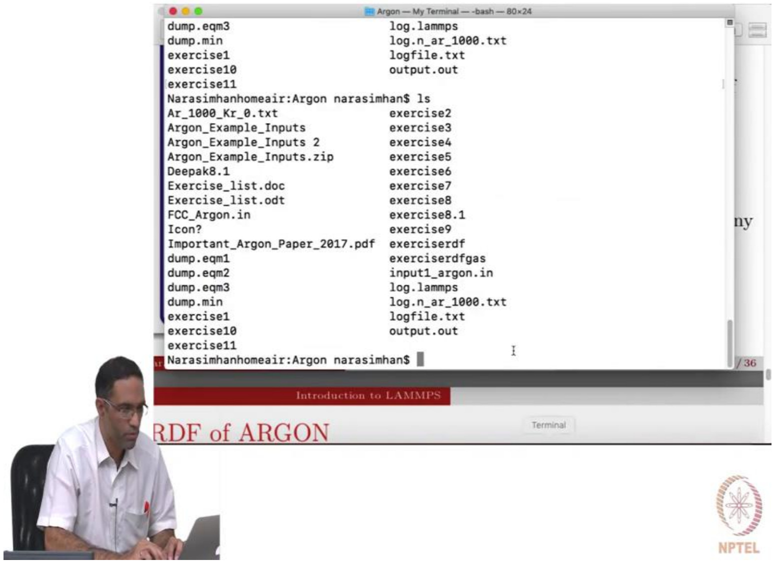
Student: Number of atoms per unit volume? So how is lammps getting that number?

Professor: It knows the number of atoms because you only created the structure, so it knows the number of atoms. It knows…

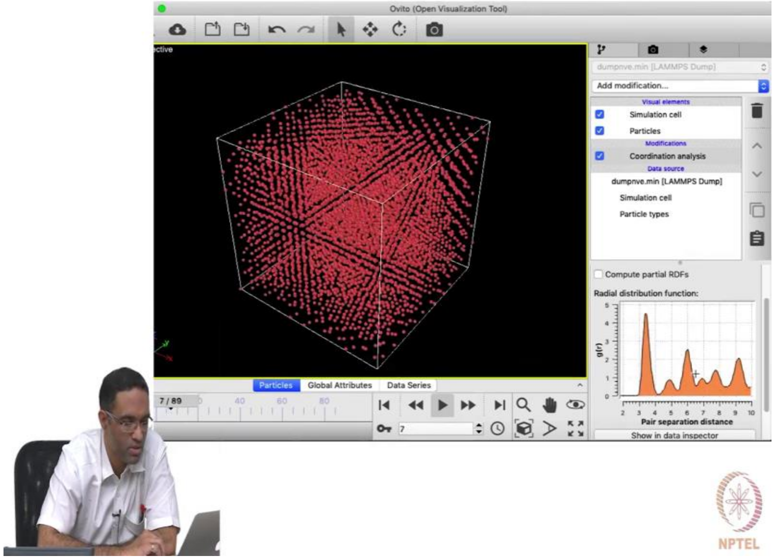
Student: And it provided the dimensions also?

Professor: Of the volume and it can also calculate the volume. Volume is variable, it is a thermodynamic variable that it can print in the thermo style, which means it knows the volume. In fact, for when you are using variables like volume, press, potential energy, kinetic energy, you do not even have to use dollar sign in order to refer to it. You can just specify volume vol and it will know that you are, you are referring to the volume of a system, press refers to the pressure.

(Refer Slide Time: 32:30)



```
dump.eqm3                          log.lammps
dump.min                           log.n_ar_1000.txt
exercise1                          logfile.txt
exercise10                         output.out
exercise11
Narasimhanhomeair:Argon narasimhan$ ls
Ar_1000_Kr_0.txt                   exercise2
Argon_Example_Inputs               exercise3
Argon_Example_Inputs 2             exercise4
Argon_Example_Inputs.zip           exercise5
Deepak8.1                          exercise6
Exercise_list.doc                  exercise7
Exercise_list.odt                  exercise8
FCC_Argon.in                       exercise8.1
Icon?                              exercise9
Important_Argon_Paper_2017.pdf     exerciserdf
dump.eqm1                          exerciserdfgas
dump.eqm2                          input1_argon.in
dump.eqm3                          log.lammps
dump.min                           log.n_ar_1000.txt
exercise1                          logfile.txt
exercise10                         output.out
exercise11
Narasimhanhomeair:Argon narasimhan$ 
```


Ovito (Open Visualization Tool)
dumpnve.min [LAMMPS Dump]
Add modification...
Visual elements
☑ Simulation cell
☑ Particles
Modifications
☑ Coordination analysis
Data source
dumpnve.min [LAMMPS Dump]
Simulation cell
Particle types
☐ Compute partial RDFs
Radial distribution function:
g(r)
Pair separation distance
Show in data inspector
Particles
Global Attributes
Data Series
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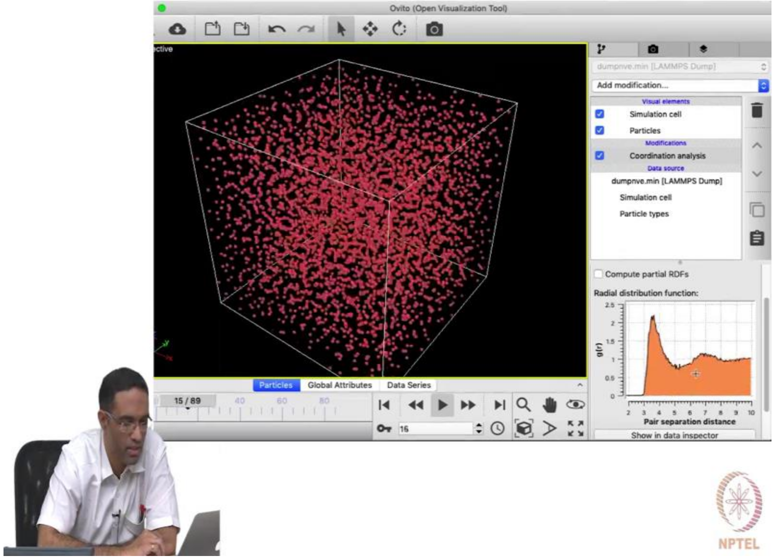
NPTEL


Ovito (Open Visualization Tool)
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Radial distribution function:
g(r)
Pair separation distance
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Particles
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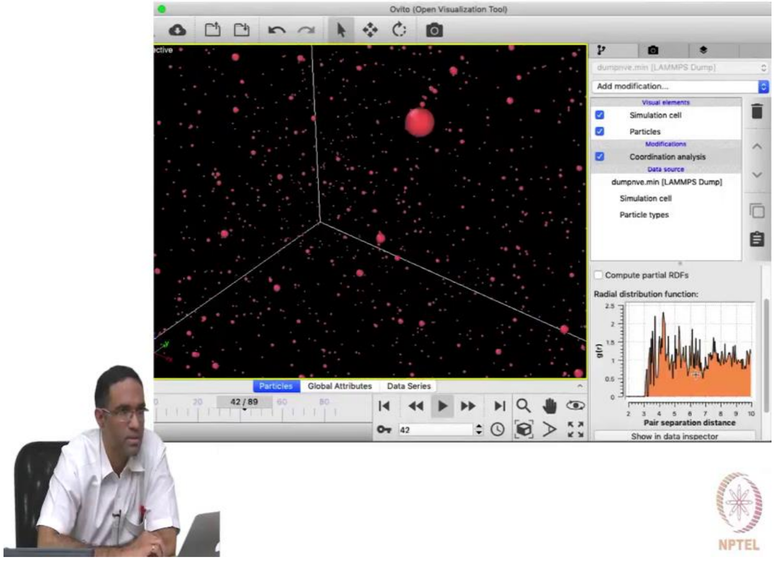

So now it is a good idea to actually see, first I do not know what is the name of the output file. So, we can reduce the size of the particle, so see how much it is expanding. So now I can actually calculate the, the pair correlation function or the g of r using right here for every time step. It is called as a coordination analysis. So you see right here, right below, it is basically point plotting exactly the same thing but it takes some time because it has to do it for every time step and it is plotting that information here. So if you start off from the beginning, but it is not doing all this averaging all that. So it starts from 1 and it has a large number of peaks.

So I can give a say smaller cutoff radius. So it is starts off with having a large number of peaks and slowly becomes something a little bit more messy and looking like a gas. So this is solid and then suddenly becomes a liquid and then gas. So this is basically useful if you want to quickly see how the structure is behaving when you are running a solution. So of course, if you want to average it, there are several ways to do it one way is to do it right from LAMMPS. And apparently now Ovito has a an ability to actually write python scripts which will allow you to average this information from Ovito itself. But you are not doing that in this course but you can explore that.

So is this RDF calculation, say the RDF calculation is just an example of global averaging. And our per and what is called velocity was example of per atom averaging. So there are so many different kinds of computes, there are so many different kinds of things that you might want to average over time. So there will be a couple of exercises that I will give you where you will encounter something that has not been done here, but I am expecting you to use the use the is whatever I have taught to actually do that correctly, check and show that you have actually understood it and then perform proper averages of the system.