Foundations of Computational Materials Modelling
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LAMMPS exercises 4

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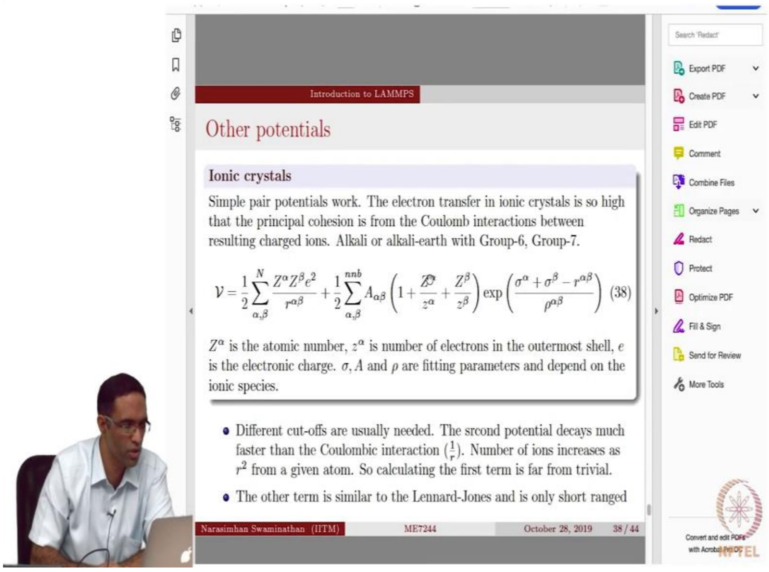

Introduction to LAMMPS

Other potentials

Ionic crystals

Simple pair potentials work. The electron transfer in ionic crystals is so high that the principal cohesion is from the Coulomb interactions between resulting charged ions. Alkali or alkali-earth with Group-6, Group-7.

$$\mathcal{V} = \frac{1}{2}\sum_{\alpha,\beta}^{N} \frac{Z^\alpha Z^\beta e^2}{r^{\alpha\beta}} + \frac{1}{2}\sum_{\alpha,\beta}^{nnb} A_{\alpha\beta}\left(1 + \frac{Z^\alpha}{z^\alpha} + \frac{Z^\beta}{z^\beta}\right)\exp\left(\frac{\sigma^\alpha + \sigma^\beta - r^{\alpha\beta}}{\rho^{\alpha\beta}}\right) \quad (38)$$

Z^α is the atomic number, z^α is number of electrons in the outermost shell, e is the electronic charge. σ, A and ρ are fitting parameters and depend on the ionic species.

- Different cut-offs are usually needed. The srcond potential decays much faster than the Coulombic interaction $(\frac{1}{r})$. Number of ions increases as r^2 from a given atom. So calculating the first term is far from trivial.
- The other term is similar to the Lennard-Jones and is only short ranged

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So, let us continue with this, these some of these exercises. So today, last class we were just looking at this potentials called as Stillinger-Weber potential. And, and we saw another potential for the ionic crystals. So, now I want to show you a simple example where Stillinger-Weber potential is used for silicon in order to say, not do anything spectacular, but simply to print the variation of the energy with for various elastic, for various Lattice parameters. So, when you plot that you should get a U-shaped curve and the value of the Lattice constant at which the energy is a minimum is basically the Lattice constant that you get for that particular material, for that potential, yeah that is the goal.

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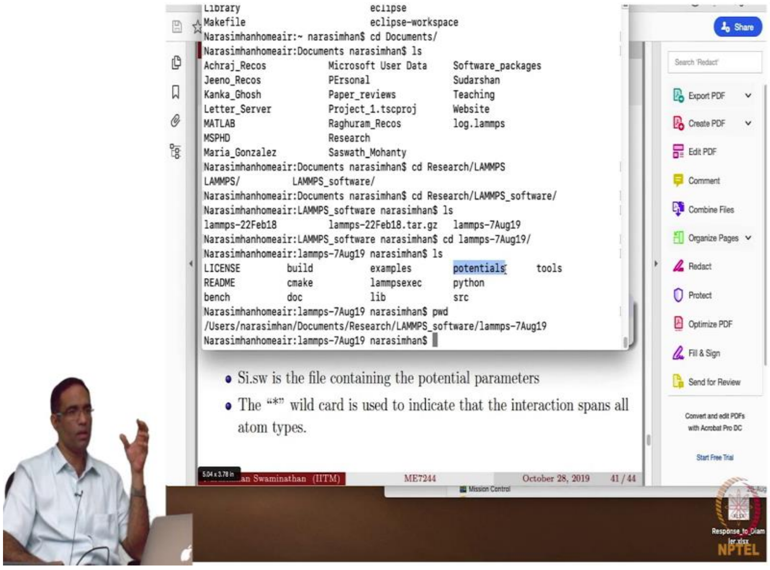
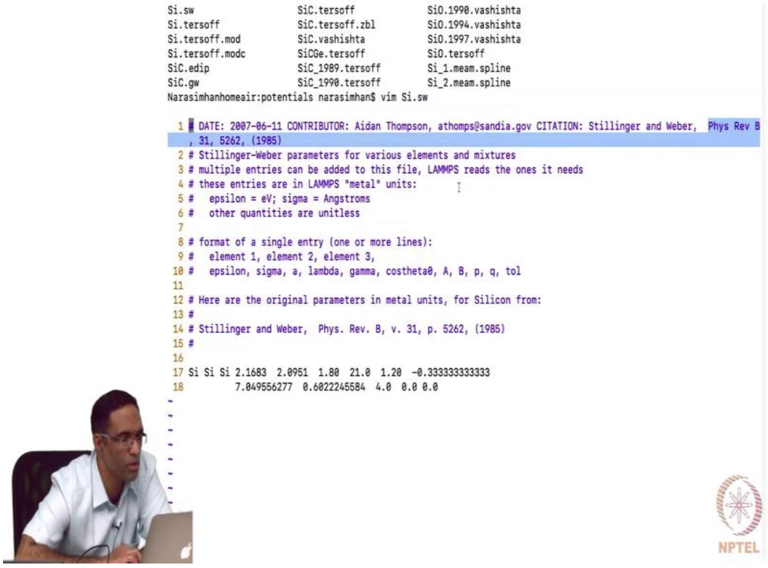


```
Library                      eclipse
Makefile                     eclipse-workspace
Narasimhanhomeair:~ narasimhan$ cd Documents/
Narasimhanhomeair:Documents narasimhan$ ls
Achraj_Recos            Microsoft User Data     Software_packages
Jeeno_Recos             PErsonal                Sudarshan
Kanka_Ghosh             Paper_reviews           Teaching
Letter_Server           Project_1.tscproj       Website
MATLAB                  Raghuram_Recos          log.lammps
MSPHD                   Research
Maria_Gonzalez          Saswath_Mohanty
Narasimhanhomeair:Documents narasimhan$ cd Research/LAMMPS
LAMMPS/          LAMMPS_software/
Narasimhanhomeair:Documents narasimhan$ cd Research/LAMMPS_software/
Narasimhanhomeair:LAMMPS_software narasimhan$ ls
lammps-22Feb18          lammps-22Feb18.tar.gz   lammps-7Aug19
Narasimhanhomeair:LAMMPS_software narasimhan$ cd lammps-7Aug19/
Narasimhanhomeair:lammps-7Aug19 narasimhan$ ls
LICENSE         build           examples        potentials      tools
README          cmake           lammpsexec      python
bench           doc             lib             src
Narasimhanhomeair:lammps-7Aug19 narasimhan$ pwd
/Users/narasimhan/Documents/Research/LAMMPS_software/lammps-7Aug19
Narasimhanhomeair:lammps-7Aug19 narasimhan$ 
```

- Si.sw is the file containing the potential parameters
- The "*" wild card is used to indicate that the interaction spans all atom types.



```
Si.sw                   SiC.tersoff             SiO.1990.vashishta
Si.tersoff              SiC.tersoff.zbl         SiO.1994.vashishta
Si.tersoff.mod          SiC.vashishta           SiO.1997.vashishta
Si.tersoff.modc         SiCGe.tersoff           SiO.tersoff
SiC.edip                SiC_1989.tersoff        Si_1.meam.spline
SiC.gw                  SiC_1990.tersoff        Si_2.meam.spline
Narasimhanhomeair:potentials narasimhan$ vim Si.sw
```

```
# DATE: 2007-06-11 CONTRIBUTOR: Aidan Thompson, athomps@sandia.gov CITATION: Stillinger and Weber,  Phys Rev B, 31, 5262, (1985)
# Stillinger-Weber parameters for various elements and mixtures
# multiple entries can be added to this file, LAMMPS reads the ones it needs
# these entries are in LAMMPS "metal" units:
#   epsilon = eV; sigma = Angstroms
#   other quantities are unitless

# format of a single entry (one or more lines):
#   element 1, element 2, element 3,
#   epsilon, sigma, a, lambda, gamma, costheta0, A, B, p, q, tol

# Here are the original parameters in metal units, for Silicon from:
#
# Stillinger and Weber,  Phys. Rev. B, v. 31, p. 5262, (1985)
#

Si Si Si 2.1683  2.0951  1.80  21.0  1.20  -0.333333333333
         7.049556277  0.6022245584  4.0  0.0 0.0
~
~
~
~
~
~
~
~
```

So, before I do that, you all should be familiar with the, the folder where LAMMPS is actually installed. So, I have installed it in some location in my computer, I have installed it right here. And if you look at it, you have the examples folder and then the potential folders. So, if you want to find out the interatomic potential for, for a specific material then you might want to start off by looking at this folder right here, a large number of potential files. And if you open one of them, say for example, this is what we are going to use, if you open them then in each of these files, you will have, you know from which article this particular potential parameters was actually taken.

So, it mean this case it was physical review B volume 31 in 1985 paper was used in order to give you the various parameters for the Stillinger-Weber potential. So, the Stillinger-Weber potential is a complicated potential with about 7 or 8 undetermined parameters which you have to give for this specific material in order for it to work. So, what we are going to do is I am just going to try to, there are several things that this exercise will do. The first thing is that it is going to, so far you have only being use the interatomic the input file. And in the input file only you described all the interatomic potential parameters also.

But now, when it comes to the potential such as the Stillinger-Weber potential, you will have to specify the potential parameters in an external file and have LAMMPS actually read the parameters from that file. A couple of things you need to keep in mind, when you are actually doing this sort of a thing, especially in the pair underscore coefficient command. The second thing is, suppose we want to do something for over a loop, over several different values of say the Lattice constant, you want it around the same file for several different Lattice constant. And then print out the energy, the Lattice constant versus the energy and make a plot of it. So, how do we do that?

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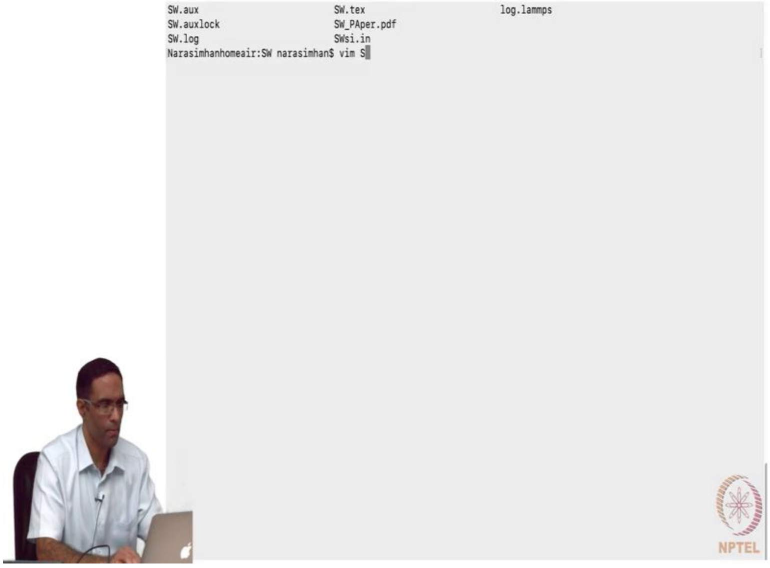
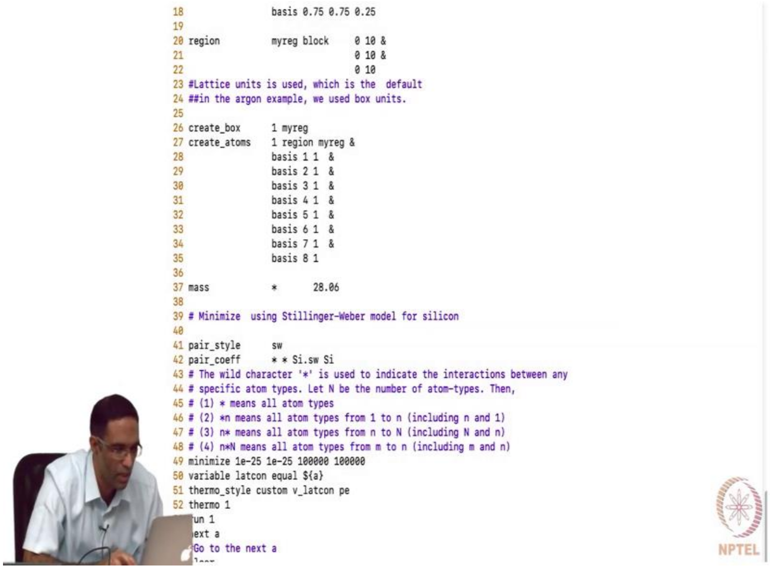


```
SW.aux                      SW.tex                      log.lammps
SW.auxlock                  SW_PAper.pdf
SW.log                      SWsi.in
Narasimhanhomeair:SW narasimhan$ vim S
```

```
# cubic diamond unit cell
variable a index 5.1 5.15 5.2 5.25 5.3 5.35 5.4 5.45 5.5 5.55 5.6 5.65 5.7 5.75 5.8 5.85
lattice         custom ${a}               &
                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 0.0 0.5 0.5       &
                basis 0.5 0.0 0.5       &
                basis 0.5 0.5 0.0       &
                basis 0.25 0.25 0.25    &
                basis 0.25 0.75 0.75    &
                basis 0.75 0.25 0.75    &
                basis 0.75 0.75 0.25

region          myreg block     0 10 &
                                0 10 &
                                0 10
#Lattice units is used, which is the  default
##in the argon example, we used box units.

create_box      1 myreg
create_atoms    1 region myreg &
                basis 1 1  &
                basis 2 1  &
                basis 3 1  &
                basis 4 1  &
                basis 5 1  &
                basis 6 1  &
                basis 7 1  &
                basis 8 1

mass            *      28.06

 Minimize  using Stillinger-Weber model for silicon

air_style       sw
```



```
                basis 0.75 0.75 0.25

region          myreg block     0 10 &
                                0 10 &
                                0 10
#Lattice units is used, which is the  default
##in the argon example, we used box units.

create_box      1 myreg
create_atoms    1 region myreg &
                basis 1 1  &
                basis 2 1  &
                basis 3 1  &
                basis 4 1  &
                basis 5 1  &
                basis 6 1  &
                basis 7 1  &
                basis 8 1

mass            *      28.06

# Minimize  using Stillinger-Weber model for silicon

pair_style      sw
pair_coeff      * * Si.sw Si
# The wild character '*' is used to indicate the interactions between any
# specific atom types. Let N be the number of atom-types. Then,
# (1) * means all atom types
# (2) *n means all atom types from 1 to n (including n and 1)
# (3) n* means all atom types from n to N (including N and n)
# (4) n*N means all atom types from m to n (including m and n)
minimize 1e-25 1e-25 100000 100000
variable latcon equal ${a}
thermo_style custom v_latcon pe
thermo 1
un 1
ext a
Go to the next a
```

So, this is going to be exercise 13, sorry exercise 12. So, I am calling my input file as SWsi dot in. So, a lot of the stuff is pretty straightforward, so the units is metal units, atom style is atomic and the periodic boundary conditions in all directions. And then what I want to do is I want to create a Lattice with some Lattice constant a. And these, these are the basis atoms for this particular material, so it is basically a diamond structure. And then define a region and then create a simulation box, create the atoms and keep calculating, minimizing, minimize the energy for that particular value of a.

And then print out the corresponding Lattice constant and the corresponding energy that I get and do this for a large number of Lattice constants. So, I defined a variable a which is of type index, which ranges from say, 5.1 through 5.85. So, all that you have to do is in the Lattice command, you say custom and instead of giving the actual value of the Lattice parameter, you just give the variable name, so just give the variable name. So, first iteration, it will have the value 5.1, everything is a same. And then I define the basis, there is only one particular type of atom here, so basis of every all the 8 atoms is just 1. The mass of the atom is given here. And then here I define the pair style, the pair style is of type sw.

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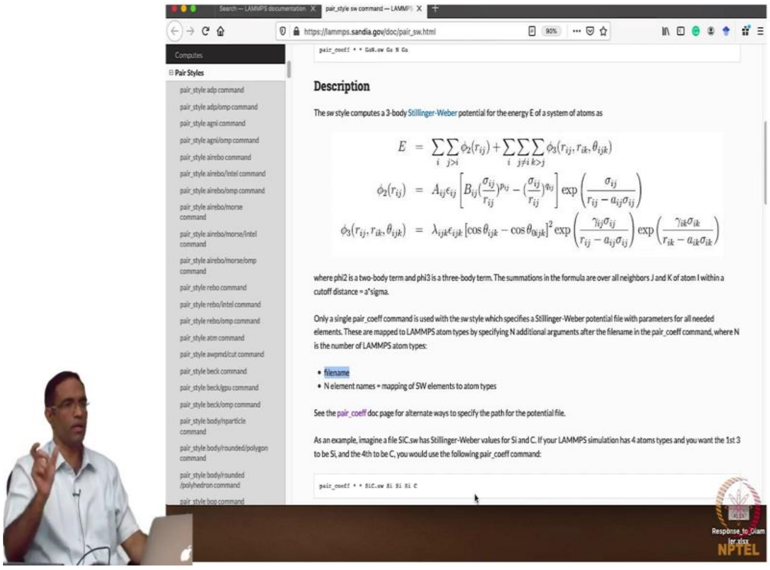


```
pair_coeff * * GaN.sw Ga N Ga
```

Description

The sw style computes a 3-body Stillinger-Weber potential for the energy E of a system of atoms as

$$E = \sum_i \sum_{j>i} \phi_2(r_{ij}) + \sum_i \sum_{j\neq i} \sum_{k>j} \phi_3(r_{ij}, r_{ik}, \theta_{ijk})$$

$$\phi_2(r_{ij}) = A_{ij}\epsilon_{ij}\left[B_{ij}\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{p_{ij}} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{q_{ij}}\right]\exp\left(\frac{\sigma_{ij}}{r_{ij} - a_{ij}\sigma_{ij}}\right)$$

$$\phi_3(r_{ij}, r_{ik}, \theta_{ijk}) = \lambda_{ijk}\epsilon_{ijk}\left[\cos\theta_{ijk} - \cos\theta_{0ijk}\right]^2 \exp\left(\frac{\gamma_{ij}\sigma_{ij}}{r_{ij} - a_{ij}\sigma_{ij}}\right)\exp\left(\frac{\gamma_{ik}\sigma_{ik}}{r_{ik} - a_{ik}\sigma_{ik}}\right)$$

where phi2 is a two-body term and phi3 is a three-body term. The summations in the formula are over all neighbors J and K of atom I within a cutoff distance = a*sigma.

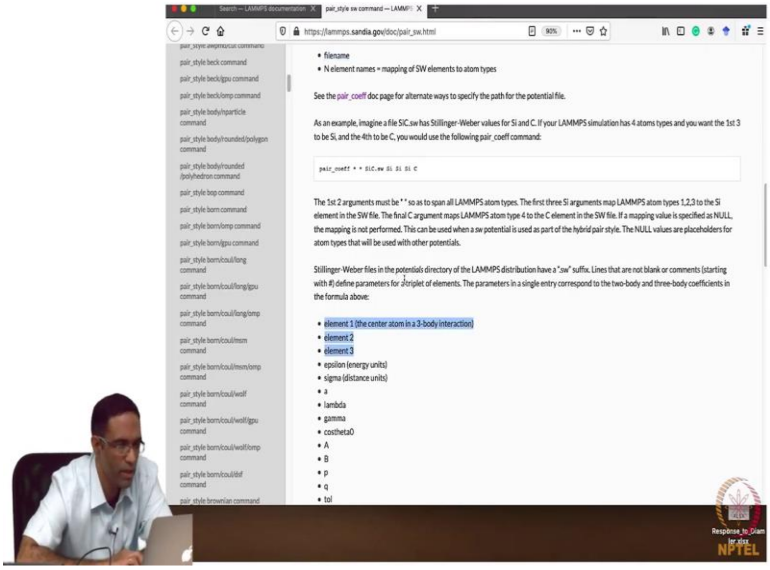
Only a single pair_coeff command is used with the sw style which specifies a Stillinger-Weber potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of SW elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential file.

As an example, imagine a file SiC.sw has Stillinger-Weber values for Si and C. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * SiC.sw Si Si Si C
```



- filename
- N element names = mapping of SW elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential file.

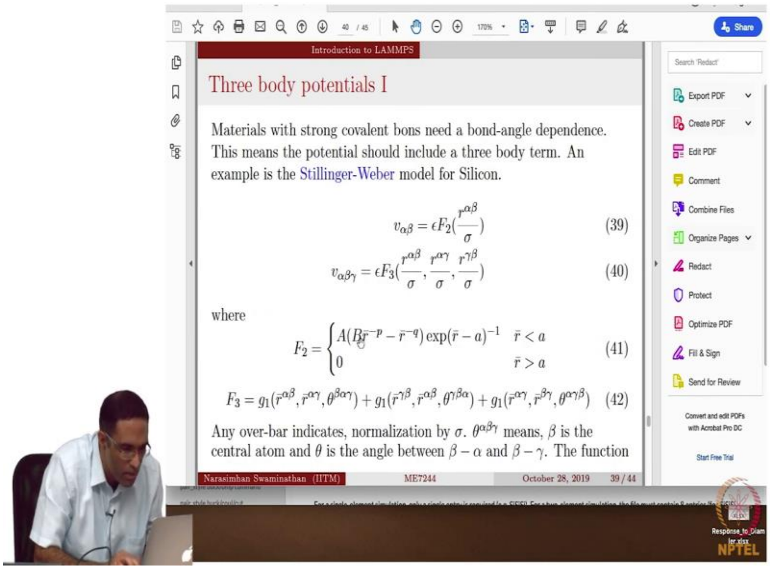
As an example, imagine a file SiC.sw has Stillinger-Weber values for Si and C. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * SiC.sw Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the SW file. The final C argument maps LAMMPS atom type 4 to the C element in the SW file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a sw potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Stillinger-Weber files in the potentials directory of the LAMMPS distribution have a ".sw" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements. The parameters in a single entry correspond to the two-body and three-body coefficients in the formula above:

- element 1 (the center atom in a 3-body interaction)
- element 2
- element 3
- epsilon (energy units)
- sigma (distance units)
- a
- lambda
- gamma
- costheta0
- A
- B
- p
- q
- tol



Three body potentials I

Materials with strong covalent bons need a bond-angle dependence. This means the potential should include a three body term. An example is the Stillinger-Weber model for Silicon.

$$v_{\alpha\beta} = \epsilon F_2(\frac{r^{\alpha\beta}}{\sigma}) \quad (39)$$

$$v_{\alpha\beta\gamma} = \epsilon F_3(\frac{r^{\alpha\beta}}{\sigma}, \frac{r^{\alpha\gamma}}{\sigma}, \frac{r^{\gamma\beta}}{\sigma}) \quad (40)$$

where

$$F_2 = \begin{cases} A(B\bar{r}^{-p} - \bar{r}^{-q}) \exp(\bar{r} - a)^{-1} & \bar{r} < a \\ 0 & \bar{r} > a \end{cases} \quad (41)$$

$$F_3 = g_1(\bar{r}^{\alpha\beta}, \bar{r}^{\alpha\gamma}, \theta^{\beta\alpha\gamma}) + g_1(\bar{r}^{\gamma\beta}, \bar{r}^{\alpha\beta}, \theta^{\gamma\beta\alpha}) + g_1(\bar{r}^{\alpha\gamma}, \bar{r}^{\beta\gamma}, \theta^{\alpha\gamma\beta}) \quad (42)$$

Any over-bar indicates, normalization by σ. $\theta^{\alpha\beta\gamma}$ means, β is the central atom and θ is the angle between $\beta - \alpha$ and $\beta - \gamma$. The function

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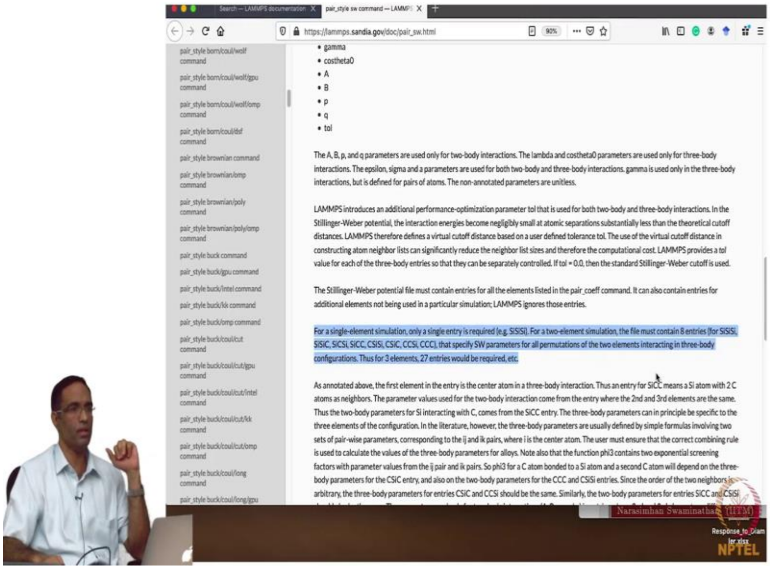

- gamma
- costheta0
- A
- B
- p
- q
- tol

The A, B, p, and q parameters are used only for two-body interactions. The lambda and costheta0 parameters are used only for three-body interactions. The epsilon, sigma and a parameters are used for both two-body and three-body interactions. gamma is used only in the three-body interactions, but is defined for pairs of atoms. The non-annotated parameters are unitless.

LAMMPS introduces an additional performance-optimization parameter tol that is used for both two-body and three-body interactions. In the Stillinger-Weber potential, the interaction energies become negligibly small at atomic separations substantially less than the theoretical cutoff distances. LAMMPS therefore defines a virtual cutoff distance based on a user defined tolerance tol. The use of the virtual cutoff distance in constructing atom neighbor lists can significantly reduce the neighbor list sizes and therefore the computational cost. LAMMPS provides a tol value for each of the three-body entries so that they can be separately controlled. If tol = 0.0, then the standard Stillinger-Weber cutoff is used.

The Stillinger-Weber potential file must contain entries for all the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries.

For a single-element simulation, only a single entry is required (e.g. SiSiSi). For a two-element simulation, the file must contain 8 entries (for SiSiSi, SiSiC, SiCSi, SiCC, CSiSi, CSiC, CCSi, CCC), that specify SW parameters for all permutations of the two elements interacting in three-body configurations. Thus for 3 elements, 27 entries would be required, etc.

As annotated above, the first element in the entry is the center atom in a three-body interaction. Thus an entry for SiCC means a Si atom with 2 C atoms as neighbors. The parameter values used for the two-body interaction come from the entry where the 2nd and 3rd elements are the same. Thus the two-body parameters for Si interacting with C, comes from the SiCC entry. The three-body parameters can in principle be specific to the three elements of the configuration. In the literature, however, the three-body parameters are usually defined by simple formulas involving two sets of pair-wise parameters, corresponding to the ij and ik pairs, where i is the center atom. The user must ensure that the correct combining rule is used to calculate the values of the three-body parameters for alloys. Note also that the function phi3 contains two exponential screening factors with parameter values from the ij pair and ik pairs. So phi3 for a C atom bonded to a Si atom and a second C atom will depend on the three-body parameters for the CSiC entry, and also on the two-body parameters for the CCC and CSiSi entries. Since the order of the two neighbors is arbitrary, the three-body parameters for entries CSiC and CCSi should be the same. Similarly, the two-body parameters for entries SiCC and CSiSi

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So, as you can see from the LAMMPS website, this is the LAMMPS website showing the expression for the energy for this 3-body Stillinger-Weber potential. And you basically need to give the name of the file which contains that tabulated values of all the constants that you have to give for this particular potential. So so, you have these elements. So, Stillinger-Weber files in the potentials directory are there, so this is this is just telling you that the potentials directory of LAMMPS has Stillinger-Weber potential and you can identify it with a dot sw suffix. But then in the actual file what is there? So, you have…

So you have, see the 3-body potential, so you need to give 3 different elements. So, depending upon what you are giving here, which order you are giving here, the parameters are going to be chosen differently from this set of values. We are doing it for a homogenous material since material with only one element type. So, for this particular case, we do not really have to worry about it. But suppose you are doing it for silicon carbide then you will have to be extremely careful. So, that is actually clearly specified here in the manual.

So, for example, if you are doing just Si Si, Si is the only thing then the first element is basically the, in the 3-body term, the first element you give is basically the one that is right in the centre. Element 2 and element 3, it could, again it is silicon-silicon in our case, because we are just simulating pure silicon then the corresponding values of epsilon, sigma, a, lambda, gamma, etcetera, etcetera. So, some of these parameters such as A, B, p and q are parameters which are going to be used only for the 2-body interactions, say, if you look at it there are so many different parameters that come here.

So, for the 2-body interactions you have A, B, p and q are the only thing that is useful parameters that are used for these 2-body interactions. Lambda cos theta naught parameters are used only for the 3-body interactions whereas the others like epsilon, sigma parameters are used for both 3-body and 2-body interactions. The most important thing is this sentence right here, so while it is specified in a very concise manner, you really have to think about it when you are actually setting up your interatomic potential file. So, for a single element simulation, you need to give only Si Si Si, it is not very complicated.

However, if your simulation contains 2 elements, say for example, silicon carbide then your every sentence in your interatomic potential file must contain an, must contain an entry and there must be 2 to the power 3 entries for each possibilities of the 3 different elements that you can have at the centre and 2 at the sides. So, you should have combinations for Si Si Si Si SiC and so on. So, we will, I will show you an input file which contains the for silicon carbide, just to illustrate how you do that. But for now, I just want to talk about the file which contains only silicon.

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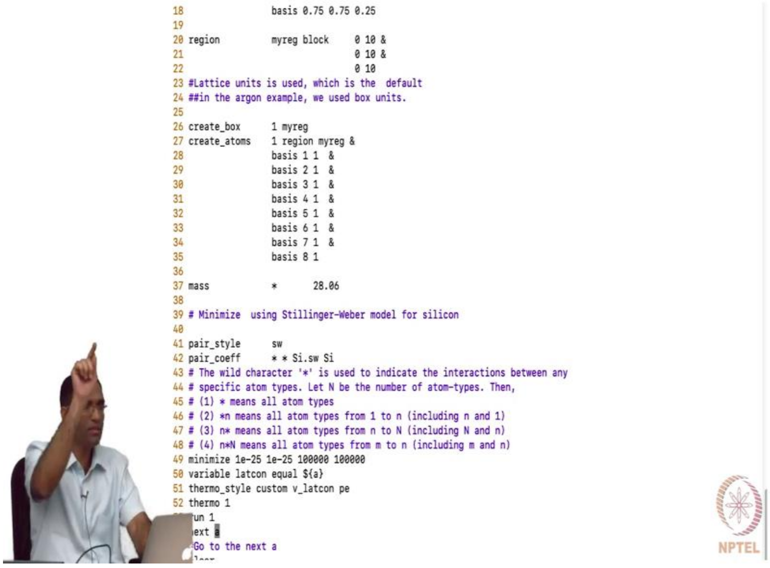

```
                basis 0.75 0.75 0.25

region          myreg block    0 10 &
                               0 10 &
                               0 10
#Lattice units is used, which is the  default
##in the argon example, we used box units.

create_box      1 myreg
create_atoms    1 region myreg &
                basis 1 1  &
                basis 2 1  &
                basis 3 1  &
                basis 4 1  &
                basis 5 1  &
                basis 6 1  &
                basis 7 1  &
                basis 8 1

mass            *      28.06

# Minimize  using Stillinger-Weber model for silicon

pair_style      sw
pair_coeff      * * Si.sw Si
# The wild character '*' is used to indicate the interactions between any
# specific atom types. Let N be the number of atom-types. Then,
# (1) * means all atom types
# (2) *n means all atom types from 1 to n (including n and 1)
# (3) n* means all atom types from n to N (including N and n)
# (4) n*N means all atom types from m to n (including m and n)
minimize 1e-25 1e-25 100000 100000
variable latcon equal ${a}
thermo_style custom v_latcon pe
thermo 1
un 1
ext a
Go to the next a
```

So, once you give these parameters right here then the pair coefficients, the pair the pair style basically specifies what is the name of the interatomic potential that we are going to use. Whereas a pair coefficient, it tells several things, it tells you what type of atoms are actually interacting, what is the file from which you can obtain these potential parameters and an elemental list which basically maps the element in the interatomic potential file to the atom type that you have chosen. So, in our case, silicon is the only atom type, so there is only one atom type present in our system. So, this Si is mapped this Si is mapped to atom type 1 in our in our simulation. Suppose we did this then, then what am I doing? I minimize the structure for this particular value of a. And then I define a new variable, variable latcon equals dollar a, basically Lattice constant is equal to the value of the a.

And then in thermo style, I print the variable latcon and the corresponding potential error, so that my thermo, so that my thermodynamic file will have their information. But when I use the thermo style, I have to do a run. If I did not do a run, nothing gets printed. So, I just say run 1, that means in once, it is just going to do 1 step and it is going to print out the corresponding Lattice constant and the potential energy that it calculated at the end of the minimization process. Then I say, next a, that means of all the a’s present here, it takes the next value of a and then I say clear and then I say jump SWsi dot in which means rerun the contents of this file. SWsi dot in is actually the name of this script, this script. So, it will rerun the contents of this script, but before doing that, you need to make sure that you have performed a clear. If you do not book clear, it will do complain.

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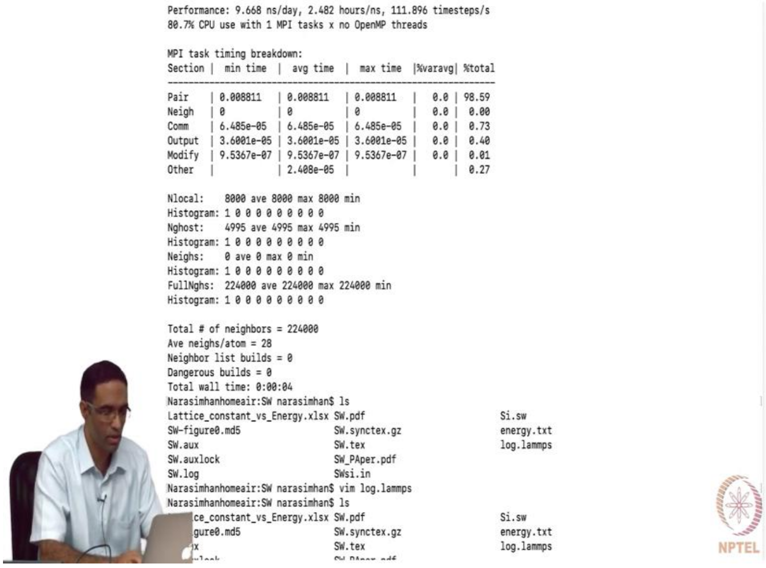
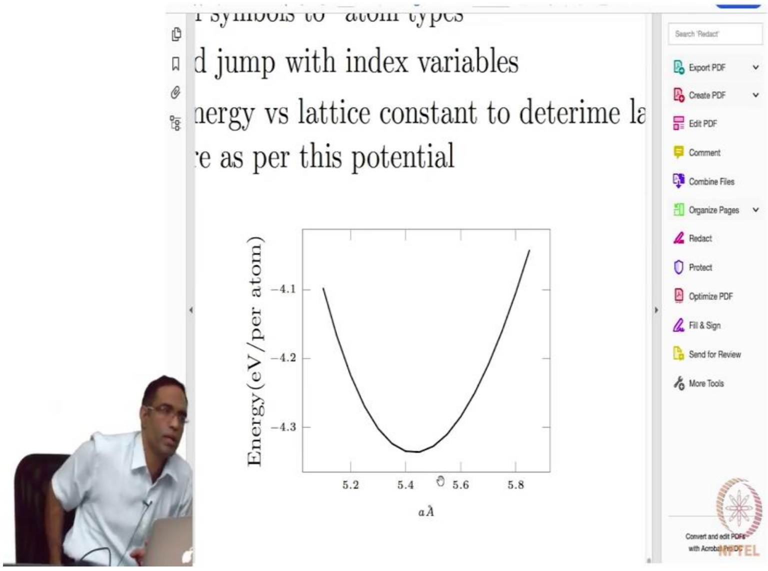


```
Performance: 9.668 ns/day, 2.482 hours/ns, 111.896 timesteps/s
80.7% CPU use with 1 MPI tasks x no OpenMP threads

MPI task timing breakdown:
Section |  min time  |  avg time  |  max time  |%varavg| %total
---------------------------------------------------------------
Pair    | 0.008811   | 0.008811   | 0.008811   |   0.0 | 98.59
Neigh   | 0          | 0          | 0          |   0.0 |  0.00
Comm    | 6.485e-05  | 6.485e-05  | 6.485e-05  |   0.0 |  0.73
Output  | 3.6001e-05 | 3.6001e-05 | 3.6001e-05 |   0.0 |  0.40
Modify  | 9.5367e-07 | 9.5367e-07 | 9.5367e-07 |   0.0 |  0.01
Other   |            | 2.408e-05  |            |       |  0.27

Nlocal:    8000 ave 8000 max 8000 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Nghost:    4995 ave 4995 max 4995 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Neighs:    0 ave 0 max 0 min
Histogram: 1 0 0 0 0 0 0 0 0 0
FullNghs:  224000 ave 224000 max 224000 min
Histogram: 1 0 0 0 0 0 0 0 0 0

Total # of neighbors = 224000
Ave neighs/atom = 28
Neighbor list builds = 0
Dangerous builds = 0
Total wall time: 0:00:04
Narasimhanhomeair:SW narasimhan$ ls
Lattice_constant_vs_Energy.xlsx SW.pdf                       Si.sw
SW-figure0.md5                  SW.synctex.gz                energy.txt
SW.aux                          SW.tex                       log.lammps
SW.auxlock                      SW_PAper.pdf
SW.log                          SWsi.in
Narasimhanhomeair:SW narasimhan$ vim log.lammps
Narasimhanhomeair:SW narasimhan$ ls
   ce_constant_vs_Energy.xlsx SW.pdf                       Si.sw
   gure0.md5                  SW.synctex.gz                energy.txt
   x                          SW.tex                       log.lammps
```



symbols to atom types

d jump with index variables

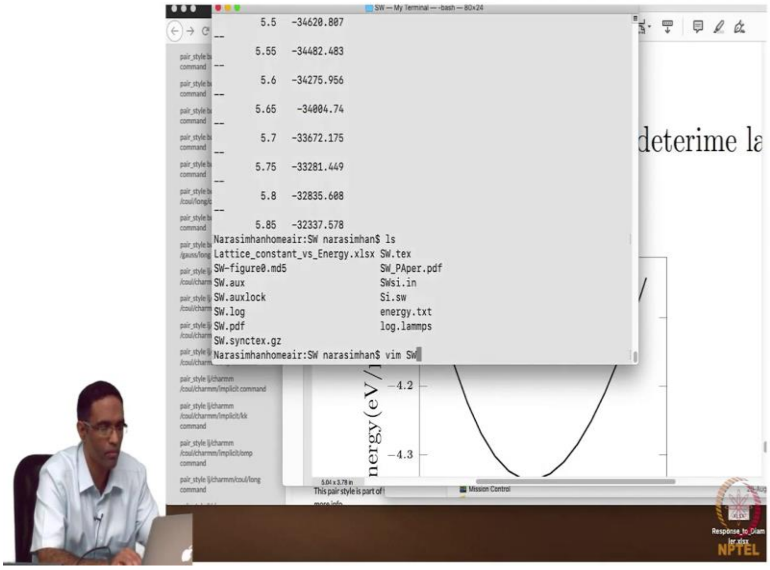
nergy vs lattice constant to deterime la

e as per this potential

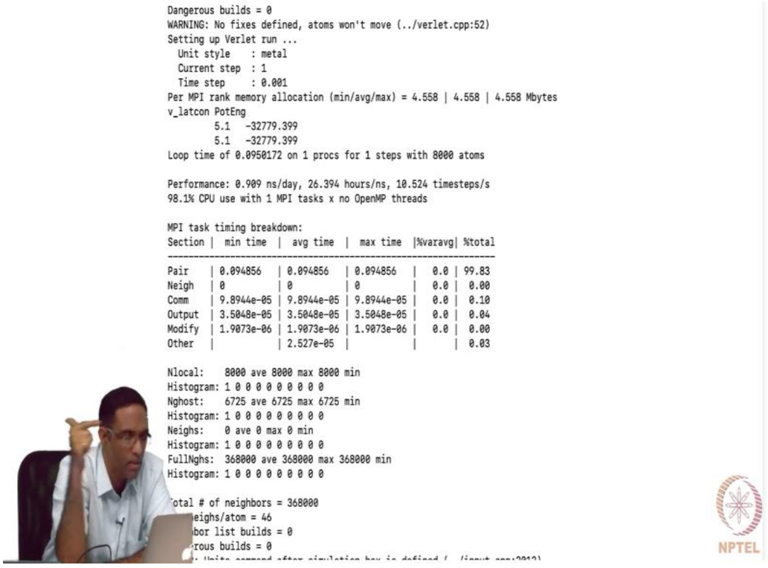
So, let us see what it does. So, let me just run it, what happens? So, it is done. So, it is giving you, its, its right for all those values of a here and if you open your logged or LAMMPS file, it is printing these potential energy for each of those Lattice parameters, which it is just of course, changing. And in all the cases, I think the minimization has just exited with energy tolerance. The energy tolerance is reached. So, it has done a good job. So now, from this you can basically extract only those lines which have the potential energy using various grep commands or any UNITS command. So, what you can do is grep, say minus a1 Pot energy logged or LAMMPS, so gives you all the line that is just after the sentence which has the string potential energy, but then I do not want this, I do not want that line either, so I again do grep minus v PotEng, so that it contains only the Lattice constant and the energies.

And then you can get rid of those dashes and basically make a plot of the energy for every Lattice parameter and you see that the Lattice parameter is, so the minimum value of the energy is obtained for some Lattice parameter between 4 and 5.4 and 5.45. So, if you check the literature, you will find out that the Lattice constant for which this potential was fitted is actually this value. So, see this this example took very few, did not take too long to run. So, all your simulations before starting on anything large, you should do such simple exercises to make sure that the values that is predicted by the interatomic potential, for which it is fitted for, somewhat reproduced by your simulations, only then we are using the interatomic potential correctly.

(Refer Slide Time: 15:00)



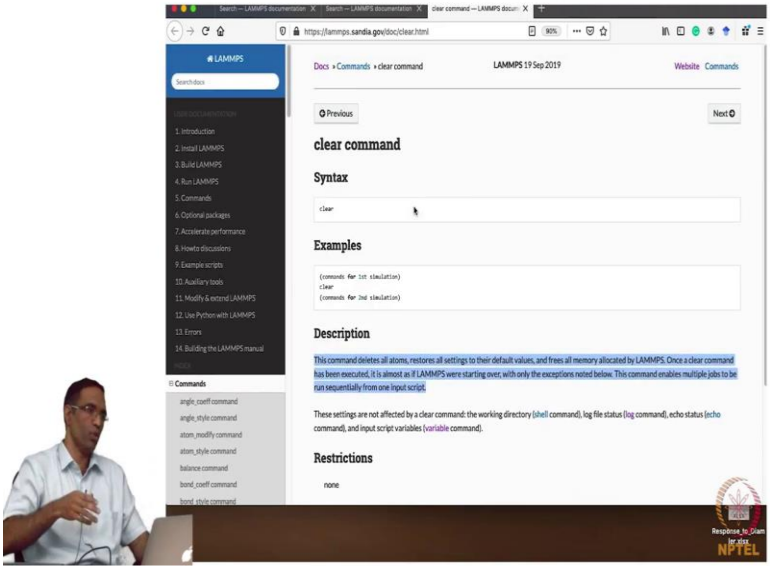
```
        5.5   -34620.807
--
       5.55   -34482.483
--
        5.6   -34275.956
--
       5.65    -34004.74
--
        5.7   -33672.175
--
       5.75   -33281.449
--
        5.8   -32835.608
--
       5.85   -32337.578
Narasimhanhomeair:SW narasimhan$ ls
Lattice_constant_vs_Energy.xlsx SW.tex
SW-figure0.md5                  SW_PAper.pdf
SW.aux                          SWsi.in
SW.auxlock                      Si.sw
SW.log                          energy.txt
SW.pdf                          log.lammps
SW.synctex.gz
Narasimhanhomeair:SW narasimhan$ vim SW
```



```
Dangerous builds = 0
WARNING: No fixes defined, atoms won't move (../verlet.cpp:52)
Setting up Verlet run ...
  Unit style    : metal
  Current step  : 1
  Time step     : 0.001
Per MPI rank memory allocation (min/avg/max) = 4.558 | 4.558 | 4.558 Mbytes
v_latcon PotEng
         5.1   -32779.399
         5.1   -32779.399
Loop time of 0.0950172 on 1 procs for 1 steps with 8000 atoms

Performance: 0.909 ns/day, 26.394 hours/ns, 10.524 timesteps/s
98.1% CPU use with 1 MPI tasks x no OpenMP threads

MPI task timing breakdown:
Section |  min time  |  avg time  |  max time  |%varavg| %total
---------------------------------------------------------------
Pair    | 0.094856   | 0.094856   | 0.094856   |   0.0 | 99.83
Neigh   | 0          | 0          | 0          |   0.0 |  0.00
Comm    | 9.8944e-05 | 9.8944e-05 | 9.8944e-05 |   0.0 |  0.10
Output  | 3.5048e-05 | 3.5048e-05 | 3.5048e-05 |   0.0 |  0.04
Modify  | 1.9073e-06 | 1.9073e-06 | 1.9073e-06 |   0.0 |  0.00
Other   |            | 2.527e-05  |            |       |  0.03

Nlocal:    8000 ave 8000 max 8000 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Nghost:    6725 ave 6725 max 6725 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Neighs:    0 ave 0 max 0 min
Histogram: 1 0 0 0 0 0 0 0 0 0
FullNghs:  368000 ave 368000 max 368000 min
Histogram: 1 0 0 0 0 0 0 0 0 0

otal # of neighbors = 368000
eighs/atom = 46
bor list builds = 0
rous builds = 0
```

Now, let us take a look what happens if you did not, so there is there are couple of things that I did there, right? So, I said clear, I said, next a. So, obviously next a is kind of clear, it just means use the next value of a. If I did not do the clear, UNITS command after simulation box is defined, so the previous run, it had defined a simulation box. When it is running again, if I did not clear the settings, it redefines the UNITS command, which is wrong. So, when you when you do clear, there are couple of things that basically is deleted from the system's memory and you are able to run a second simulation.

(Refer Slide Time: 15:55)



clear command

Syntax

```
clear
```

Examples

```
(commands for 1st simulation)
clear
(commands for 2nd simulation)
```

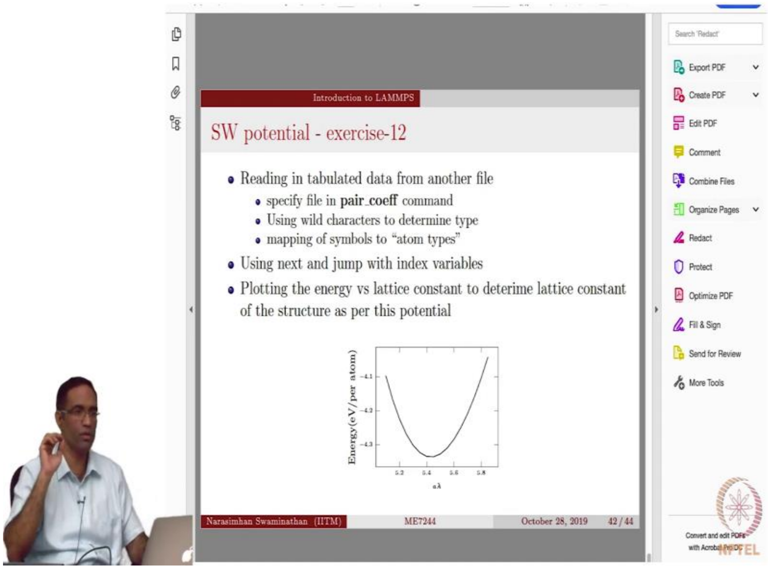
Description

This command deletes all atoms, restores all settings to their default values, and frees all memory allocated by LAMMPS. Once a clear command has been executed, it is almost as if LAMMPS were starting over, with only the exceptions noted below. This command enables multiple jobs to be run sequentially from one input script.

These settings are not affected by a clear command: the working directory (shell command), log file status (log command), echo status (echo command), and input script variables (variable command).

Restrictions

none



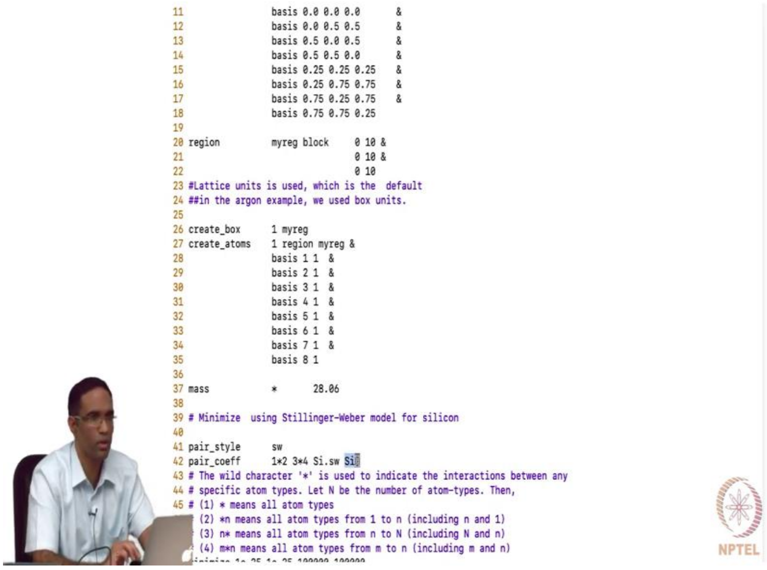
SW potential - exercise-12

- Reading in tabulated data from another file
  - specify file in **pair_coeff** command
  - Using wild characters to determine type
  - mapping of symbols to "atom types"
- Using next and jump with index variables
- Plotting the energy vs lattice constant to deterime lattice constant of the structure as per this potential

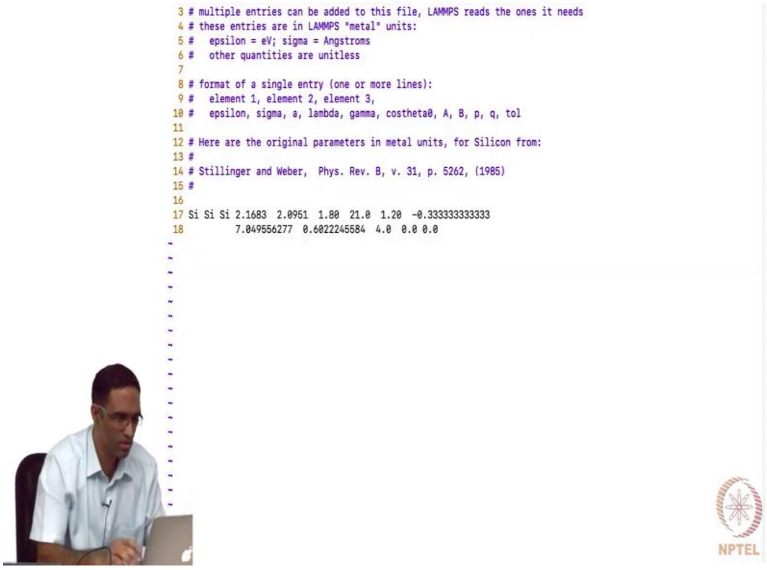
So, basically what it does is something very specific. See, this command deletes all atoms, restores all settings to their default values and frees all the memory allocated by LAMMPS. Once a clear command is executed, it is almost as if LAMMPS were starting over again with only the exceptions not addressed. So, there are exceptions, which means the variable and all is not deleted. It still remembers what the next a is. This command enables multiple jobs to be run sequentially from one input script. These settings are not affected by the clear command, the working directory shell command, log file status, echo status and input script variables which is basically the variable command. So, this is extremely useful. Once you know how to do stuff in a loop, you can run your simulations for various temperatures, for various pressure.

So, that is one thing that I wanted to demonstrate here. So, this is the example with this Stilling-Weber potential and the pair coefficients in this particular case just had an wild character basically saying that you have to span all possible atom types for which I am giving you the interatomic potential file here. But it is possible that your interatomic potential might require interaction between atoms of different types, for example, if you were going to simulate the interactions of ideal gas containing argon and krypton, so Kr atom type 1 and atom type, 2 then you would have to have interactions between argon argon, krypton krypton and argon krypton. And then they have different values, they will have different values.

(Refer Slide Time: 17:43)



```
               basis 0.0 0.0 0.0       &
               basis 0.0 0.5 0.5       &
               basis 0.5 0.0 0.5       &
               basis 0.5 0.5 0.0       &
               basis 0.25 0.25 0.25    &
               basis 0.25 0.75 0.75    &
               basis 0.75 0.25 0.75    &
               basis 0.75 0.75 0.25

region         myreg block     0 10 &
                               0 10 &
                               0 10
#Lattice units is used, which is the  default
##in the argon example, we used box units.

create_box     1 myreg
create_atoms   1 region myreg &
               basis 1 1  &
               basis 2 1  &
               basis 3 1  &
               basis 4 1  &
               basis 5 1  &
               basis 6 1  &
               basis 7 1  &
               basis 8 1

mass           *       28.06

# Minimize  using Stillinger-Weber model for silicon

pair_style     sw
pair_coeff     1*2 3*4 Si.sw Si
# The wild character '*' is used to indicate the interactions between any
# specific atom types. Let N be the number of atom-types. Then,
# (1) * means all atom types
# (2) *n means all atom types from 1 to n (including n and 1)
# (3) n* means all atom types from n to N (including N and n)
# (4) m*n means all atom types from m to n (including m and n)
```



```
# multiple entries can be added to this file, LAMMPS reads the ones it needs
# these entries are in LAMMPS "metal" units:
#   epsilon = eV; sigma = Angstroms
#   other quantities are unitless

# format of a single entry (one or more lines):
#   element 1, element 2, element 3,
#   epsilon, sigma, a, lambda, gamma, costheta0, A, B, p, q, tol

# Here are the original parameters in metal units, for Silicon from:
#
# Stillinger and Weber,  Phys. Rev. B, v. 31, p. 5262, (1985)
#

Si Si Si 2.1683  2.0951  1.80  21.0  1.20  -0.333333333333
         7.049556277  0.6022245584  4.0  0.0 0.0
```

So, for each and every possible pairs, you will have to specify the corresponding pair coefficient the atom types there. So, so here, each star means all atom types, between all atom types. But star n means all atom types from 1 through n, including n and 1, n star means all atoms types from small n to capital N, where N is a (total) capital N is total number of atom types. So, n star N means all atom types from m to n. Sorry this should be m to n. So, so you can give here something like this.

So, there are 4 atom types, interactions between atoms of type 1 to 2 with interactions of atoms of type 3 to 4 are going to have some set of coefficients here. It is not applicable for this example, but imagine your Lennard-Jones case where you actually specify epsilon and sigma and the corresponding cut-off. So, instead of choosing each and every one, suppose you had 20 different atom types, then you could in principle do something 1 to 10, 11 to 20 to describe the interactions between 1 through 10, all atom types are 1 through 10 with all atom types of spanning from 11 through 20. Of course, you will have to give other interactions as well, this is just one set.

Student: It should be 10 power 10, 10 power 10.

Professor: But, 10 power 10 interactions, possible this is just an example. So, let us give one, seems huge. So, 1 to 2, 2 to 4, 3 to 4.

Student: So, if I…

Professor: Yes.

Student: If I am making this command…

Professor: No that is what to give those many, the idea is to give so many interactions, you do not have to like type each and every pair is what, this command helps you do. If they are having the same set of sigma epsilon values.

Student: Oh, so this is only for one particular sigma.

Professor: Yeah, yeah, exactly.

Student: So, they are changing every line?

Professor: You have to give a additional lines with the corresponding pair coefficients. You have to add other pair coefficients to take care of other interactions.

Student: When you repeat from a file that, so will it match on its own?

Professor: It will not match on its own. You have to give what element you are matching to. So, for example in this case the Si that you are giving here, the Si that you are giving here is actually the same label that appears in the potential file here, this label that is appearing here. So, that could be a and this could be a a a. Because it appears first, that element Si or a a is going to be mapped to atom type 1.

(Refer Slide Time: 21:10)

```
lattice        custom ${a}             &
               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 0.0 0.5 0.5      &
               basis 0.5 0.0 0.5      &
               basis 0.5 0.5 0.0      &
               basis 0.25 0.25 0.25   &
               basis 0.25 0.75 0.75   &
               basis 0.75 0.25 0.75   &
               basis 0.75 0.75 0.25

region         myreg block     0 10 &
                               0 10 &
                               0 10
#Lattice units is used, which is the  default
##in the argon example, we used box units.

create_box     8 myreg
create_atoms   1 region myreg &
               basis 1 1  &
               basis 2 2  &
               basis 3 3  &
               basis 4 4  &
               basis 5 5  &
               basis 6 6  &
               basis 7 7  &
               basis 8 8

mass           *      28.06

# Minimize  using Stillinger-Weber model for silicon

pair_style     sw
air_coeff      * * Si.sw Si Si Si Si Si Si Si Si
 The wild character '*' is used to indicate the interactions between any
 specific atom types. Let N be the number of atom-types. Then,
```

So, what this means is one, one more way of explaining this is to actually, say it for example, just for the heck of it, 8, it works. So so, there are 8 atom types, I just set there are 8 atom types, did you see that? I just set, there 8 atom types, basis atom 1 is of type 1, basis atom 2 is of type 2, basis atom 3 is of type 3, I I just set that and then I just set my in my pair coefficient, this is Si dot sw is the name of the file and each of these labels Si should map to the corresponding type that it is, that is generated. So, each of this is a, so you can imagine if it is more than 1.

So, if it is silicon carbide then you would, if in your input file, you you modelled Si to be of type 1 and C to be of type 2 then you would do this, but you can also do this provided you keep track of which basis is carbon and which basis is basically silica. Now, this is easier set than dump, it can get really, really confusing when you are actually doing it for these multibody potential. So, I will try to give you an example where we have, we do a test of potential where exactly the same type of input file actually has to be given.

Student: Sir if…

Professor: Yeah?

Student: If I use 1 star 2 and 3 star 4, does it mean that…

Professor: What is it, what is it? If I use?

Student: Pair coefficient, I use 1star 2 and 3 star 4.

Professor: 1 star 2 and?

Student: 3 star 4, does it mean it includes only the interaction between 1 and 2 and 3 and 4?

Professor: No. 1 2 and 3 4. All atoms of types 1 through 2 including 1 and 2 with all atoms of type 3 to 4 including 3 and 4.

Student: So, it includes 1 3, 1 4, 2 3?

Professor: 2 3, 2 4, yes.

Student: So, it does not include 1 with 2?

Professor: Yes, you would have to give that, yes.

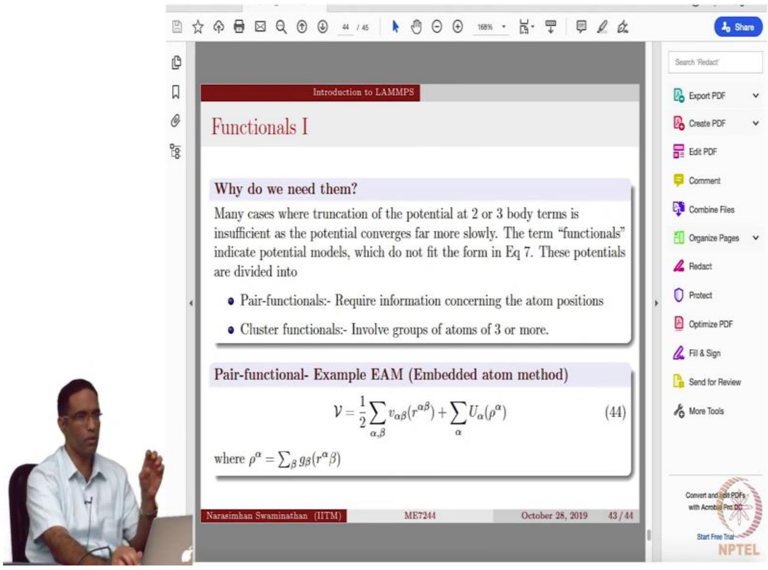
Student: Sir, for, for this particular, can write this code? We should know what, what the structure of that file is. It is due to the same label.

Professor: Label, yes, yes. We are generating that label, you are, actually you are generating that file.

Student: But in this case, we took it…

Professor: We took it for, otherwise you will have to generate. You could call it A,B,C and put A,B,C here, it should be it should work fine.

(Refer Slide Time: 24:31)



Introduction to LAMMPS

Functionals I

Why do we need them?

Many cases where truncation of the potential at 2 or 3 body terms is insufficient as the potential converges far more slowly. The term "functionals" indicate potential models, which do not fit the form in Eq 7. These potentials are divided into

- Pair-functionals:- Require information concerning the atom positions
- Cluster functionals:- Involve groups of atoms of 3 or more.

Pair-functional- Example EAM (Embedded atom method)

$$\mathcal{V} = \frac{1}{2}\sum_{\alpha,\beta} v_{\alpha\beta}(r^{\alpha\beta}) + \sum_{\alpha} U_{\alpha}(\rho^{\alpha}) \qquad (44)$$

where $\rho^{\alpha} = \sum_{\beta} g_{\beta}(r^{\alpha}\beta)$

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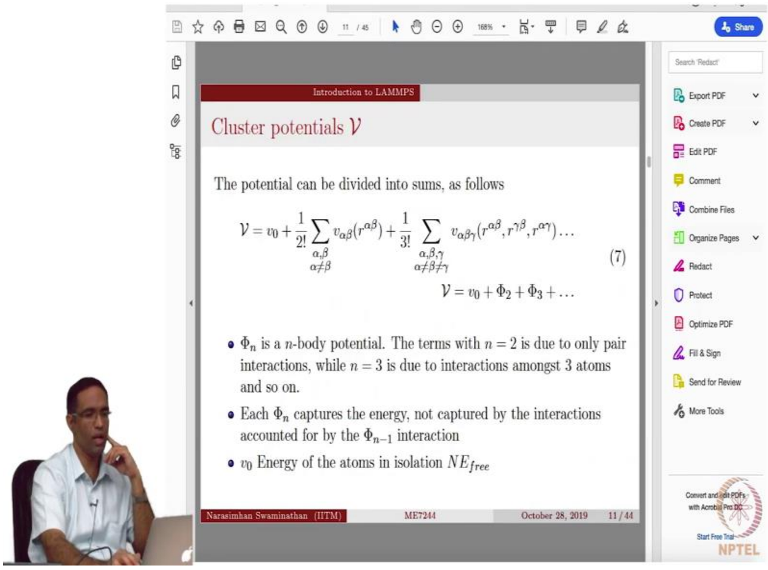

Introduction to LAMMPS

Cluster potentials $\mathcal{V}$

The potential can be divided into sums, as follows

$$\mathcal{V} = v_0 + \frac{1}{2!}\sum_{\substack{\alpha,\beta \\ \alpha\neq\beta}} v_{\alpha\beta}(r^{\alpha\beta}) + \frac{1}{3!}\sum_{\substack{\alpha,\beta,\gamma \\ \alpha\neq\beta\neq\gamma}} v_{\alpha\beta\gamma}(r^{\alpha\beta}, r^{\gamma\beta}, r^{\alpha\gamma})\ldots \qquad (7)$$

$$\mathcal{V} = v_0 + \Phi_2 + \Phi_3 + \ldots$$

- Φ_n is a n-body potential. The terms with $n = 2$ is due to only pair interactions, while $n = 3$ is due to interactions amongst 3 atoms and so on.
- Each Φ_n captures the energy, not captured by the interactions accounted for by the Φ_{n-1} interaction
- v_0 Energy of the atoms in isolation NE_{free}

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Now, another important form of interatomic potential is basically the embedded atom method. So, the problem is, see now all of these examples that I am giving you, I am just going to do how to specify the interatomic potential file and do a simple, plot the Lattice constant versus energy, because minimization and doing other exercises on that is kind of similar to what we have done for argon. At least the kind of fixes that you must use, all those things remain pretty much the same.

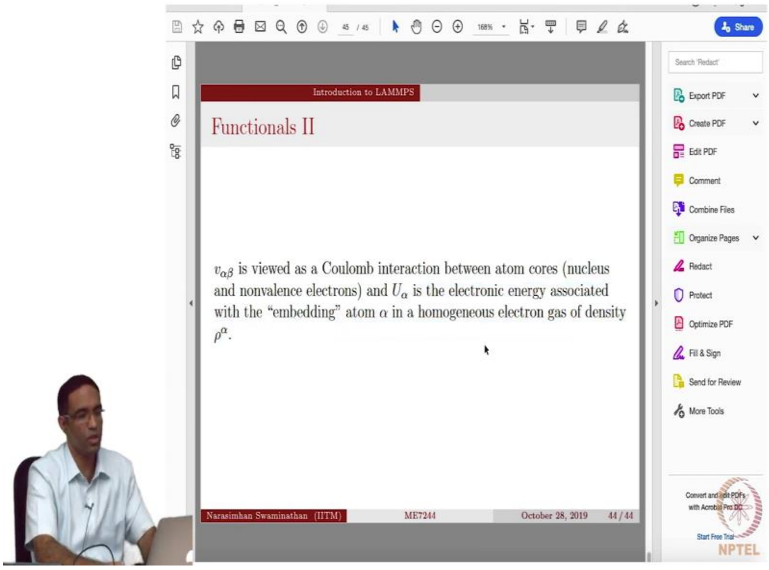
So, why do you need, there are other kinds of, right now whatever we talked about were called potentials, pair potentials which basically, a pair potentials or 3-body potentials which basically was a reflection of the fact that we could truncate our interatomic potential at some point. So, this is 2-body, this is the 3-body and then you have the 4-body and so on. We just said that anything after this is actually not important and we stop with it. So, we did Lennard-Jones 2-body and then Stilling-Weber's 3-body potential. But it so happens that for some in some cases like metals, these the higher body potentials do not converge quickly to a value.

So, you really cannot neglect all the higher, higher order potentials so to speak. But it is also inconvenient to use all the higher order potentials for obvious reasons, you have more combinations of r alpha beta to actually take in to account. And it is very difficult to come up with functional forms that will actually do this. So, people have come up with something referred to as functionals. The name functional is used wherever the interatomic potential form does not appear like what it does, here it is called a cluster potential, does not appear like this. The functional form does not appear like this then it is called a functional.

The interatomic potential form of the function does not look like that, so it is called as a functional. And you can, there are interatomic models which are actually not looking like that and they are classified into 2 categories, one is pair functionals and other is cluster functionals. So, pair functionals, as you can imagine require only, they still require only distance information, but the functional form will not look like that and cluster functional involves group of 3 or more atoms. So, an example of the embedded atom potential is like this, which is very commonly used for metals.

Embedded atoms, so it is kind of capturing the fact that your atom is actually embedded in a sea of electrons. So, basically the energy depends upon the energy of the electron gas that is basically surrounding the atom. So, that is the basic idea, of course there is a lot of physics as to why that form of interatomic potential is appropriate for such systems, we are not going to deal, deal with that. We just want to know, what this embedded atom does and approximately somewhat understand how to use it when you are trying to do simulations with LAMMPS. So, embedded atom method, this is the functional form, it consists of a pair function plus the embedding energy term, which depends on rho alpha which is again the local density of the electron gas.

(Refer Slide Time: 28:17)



Introduction to LAMMPS

Functionals II

$v_{\alpha\beta}$ is viewed as a Coulomb interaction between atom cores (nucleus and nonvalence electrons) and U_α is the electronic energy associated with the "embedding" atom α in a homogeneous electron gas of density ρ^α.

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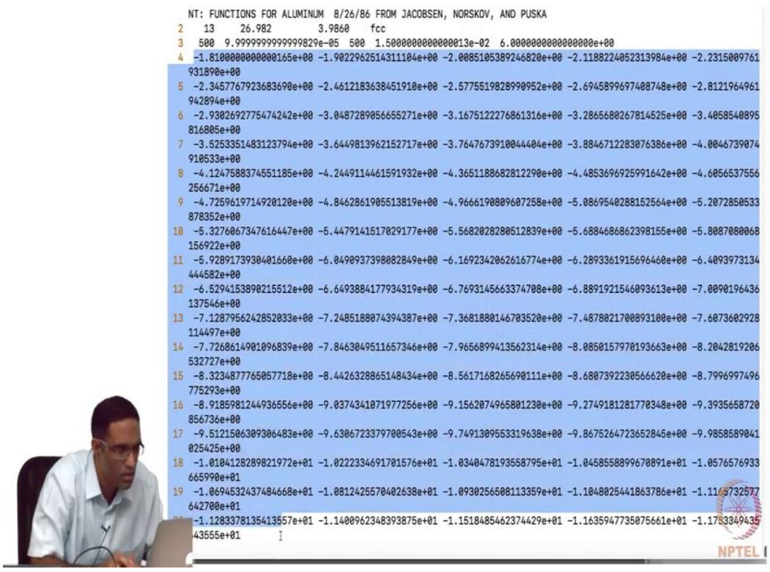
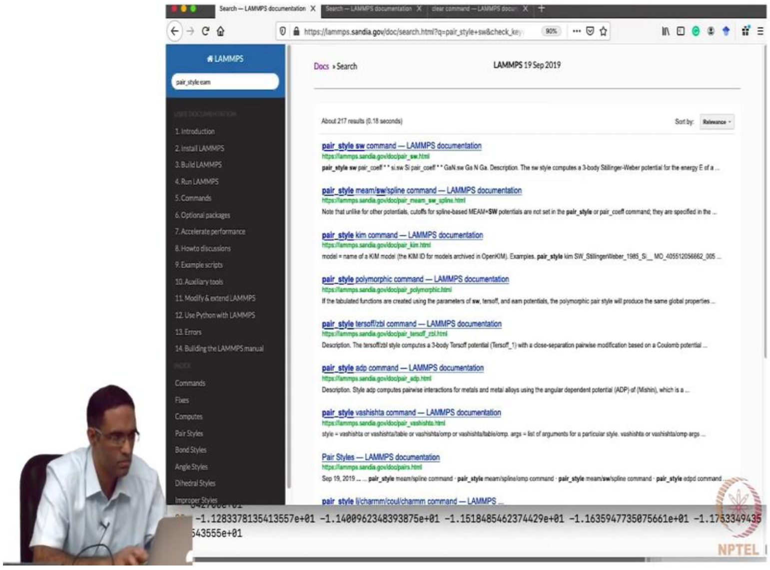
So so, v alpha is viewed as a Coulomb interaction between atom but it is not actually z alpha, z beta and all that, something else. And U alpha is the electronic energy associated with the embedding of the atom alpha in a sea of electron or electron gas of density rho alpha, so that is what this is.

(Refer Slide Time: 28:40)



```
NT: FUNCTIONS FOR ALUMINUM  8/26/86 FROM JACOBSEN, NORSKOV, AND PUSKA
  13    26.982         3.9860    fcc
 500  9.9999999999999829e-05  500  1.5000000000000013e-02  6.0000000000000000e+00
 -1.8100000000000165e+00 -1.9022962514311104e+00 -2.0085105389246820e+00 -2.1188224052313984e+00 -2.2315009761
931890e+00
 -2.3457767923683690e+00 -2.4612183638451910e+00 -2.5775519828990952e+00 -2.6945899697408748e+00 -2.8121964961
942894e+00
 -2.9302692775474242e+00 -3.0487289056655271e+00 -3.1675122276861316e+00 -3.2865680267814525e+00 -3.4058540895
816805e+00
 -3.5253351483123794e+00 -3.6449813962152717e+00 -3.7647673910044404e+00 -3.8846712283076386e+00 -4.0046739074
910533e+00
 -4.1247588374551185e+00 -4.2449114461591932e+00 -4.3651188682812290e+00 -4.4853696925991642e+00 -4.6056537556
256671e+00
 -4.7259619714920120e+00 -4.8462861905513819e+00 -4.9666190809607258e+00 -5.0869540288152564e+00 -5.2072850533
878352e+00
 -5.3276067347616447e+00 -5.4479141517029177e+00 -5.5682028280512839e+00 -5.6884686862398155e+00 -5.8087080068
156922e+00
 -5.9289173930401660e+00 -6.0490937398082849e+00 -6.1692342062616774e+00 -6.2893361915696460e+00 -6.4093973134
444582e+00
 -6.5294153890215512e+00 -6.6493884177934319e+00 -6.7693145663374708e+00 -6.8891921546093613e+00 -7.0090196436
137546e+00
 -7.1287956242852033e+00 -7.2485188074394387e+00 -7.3681880146703520e+00 -7.4878021700893100e+00 -7.6073602928
114497e+00
 -7.7268614901096839e+00 -7.8463049511657346e+00 -7.9656899413562314e+00 -8.0850157970193663e+00 -8.2042819206
532727e+00
 -8.3234877765057718e+00 -8.4426328865148434e+00 -8.5617168265690111e+00 -8.6807392230566620e+00 -8.7996997496
775293e+00
 -8.9185981244936556e+00 -9.0374341071977256e+00 -9.1562074965801230e+00 -9.2749181281770348e+00 -9.3935658720
856736e+00
 -9.5121506309306483e+00 -9.6306723379700543e+00 -9.7491309553319638e+00 -9.8675264723652845e+00 -9.9858589041
025425e+00
 -1.0104128289821972e+01 -1.0222334691701576e+01 -1.0340478193558795e+01 -1.0458558899670891e+01 -1.0576576933
665990e+01
 -1.0694532437484668e+01 -1.0812425570402638e+01 -1.0930256508113359e+01 -1.1048025441863786e+01 -1.1165732577
642700e+01
 -1.1283378135413557e+01 -1.1400962348393875e+01 -1.1518485462374429e+01 -1.1635947735075661e+01 -1.1753349435
43555e+01
```



Docs » Search

LAMMPS 19 Sep 2019

About 217 results (0.18 seconds)

pair_style sw command — LAMMPS documentation
https://lammps.sandia.gov/doc/pair_**sw**.html
pair_style sw pair_coeff * * si.sw Si pair_coeff * * GaN.sw Ga N Ga. Description. The sw style computes a 3-body Stillinger-Weber potential for the energy E of a ...

pair_style meam/**sw**/spline command — LAMMPS documentation
https://lammps.sandia.gov/doc/pair_meam_**sw**_spline.html
Note that unlike for other potentials, cutoffs for spline-based MEAM+**SW** potentials are not set in the **pair_style** or pair_coeff command; they are specified in the ...

pair_style kim command — LAMMPS documentation
https://lammps.sandia.gov/doc/pair_kim.html
model = name of a KIM model (the KIM ID for models archived in OpenKIM). Examples. **pair_style** kim SW_StillingerWeber_1985_Si__MO_405512056662_005 ...

pair_style polymorphic command — LAMMPS documentation
https://lammps.sandia.gov/doc/pair_polymorphic.html
If the tabulated functions are created using the parameters of **sw**, tersoff, and eam potentials, the polymorphic pair style will produce the same global properties ...

pair_style tersoff/zbl command — LAMMPS documentation
https://lammps.sandia.gov/doc/pair_tersoff_zbl.html
Description. The tersoff/zbl style computes a 3-body Tersoff potential (Tersoff_1) with a close-separation pairwise modification based on a Coulomb potential ...

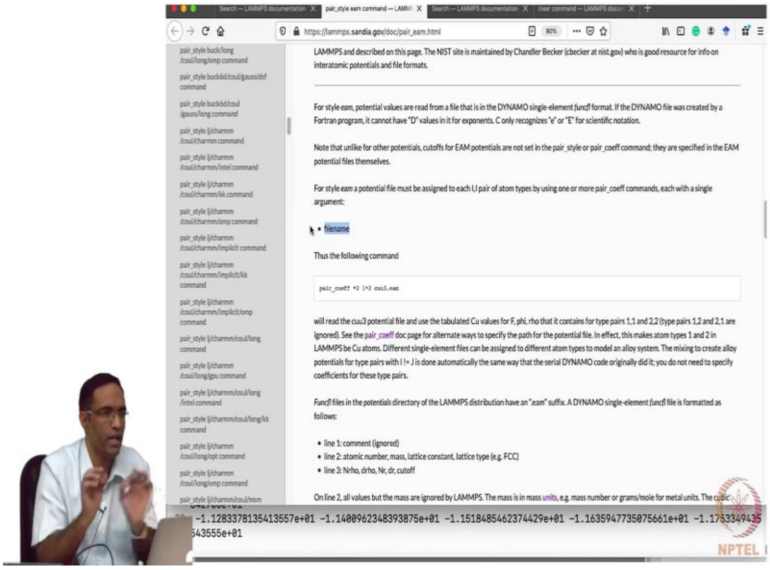
pair_style adp command — LAMMPS documentation
https://lammps.sandia.gov/doc/pair_adp.html
Description. Style adp computes pairwise interactions for metals and metal alloys using the angular dependent potential (ADP) of (Mishin), which is a ...

pair_style vashishta command — LAMMPS documentation
https://lammps.sandia.gov/doc/pair_vashishta.html
style = vashishta or vashishta/table or vashishta/omp or vashishta/table/omp. args = list of arguments for a particular style. vashishta or vashishta/omp args ...

Pair Styles — LAMMPS documentation
https://lammps.sandia.gov/doc/pairs.html
Sep 19, 2019 ... ... **pair_style** meam/spline command · **pair_style** meam/spline/omp command · **pair_style** meam/**sw**/spline command · **pair_style** edpd command ...

pair_style lj/charmm/coul/charmm command — LAMMPS ...

```
 -1.1283378135413557e+01 -1.1400962348393875e+01 -1.1518485462374429e+01 -1.1635947735075661e+01 -1.1753349435
543555e+01
```



LAMMPS and described on this page. The NIST site is maintained by Chandler Becker (cbecker at nist.gov) who is good resource for info on interatomic potentials and file formats.

For style *eam*, potential values are read from a file that is in the DYNAMO single-element *funcfl* format. If the DYNAMO file was created by a Fortran program, it cannot have "D" values in it for exponents. C only recognizes "e" or "E" for scientific notation.

Note that unlike for other potentials, cutoffs for EAM potentials are not set in the pair_style or pair_coeff command; they are specified in the EAM potential files themselves.

For style *eam* a potential file must be assigned to each I,I pair of atom types by using one or more pair_coeff commands, each with a single argument:

- filename

Thus the following command

```
pair_coeff *2 1*2 cuu3.eam
```

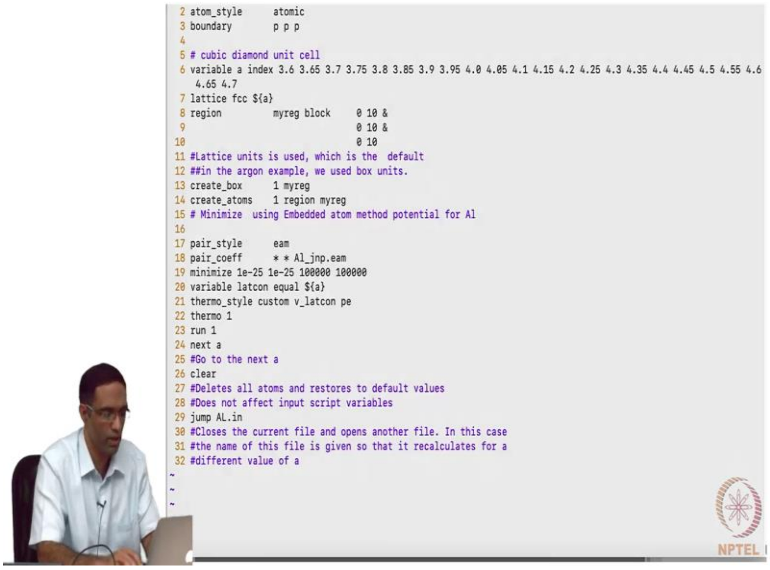
will read the cuu3 potential file and use the tabulated Cu values for F, phi, rho that it contains for type pairs 1,1 and 2,2 (type pairs 1,2 and 2,1 are ignored). See the pair_coeff doc page for alternate ways to specify the path for the potential file. In effect, this makes atom types 1 and 2 in LAMMPS be Cu atoms. Different single-element files can be assigned to different atom types to model an alloy system. The mixing to create alloy potentials for type pairs with I != J is done automatically the same way that the serial DYNAMO code originally did it; you do not need to specify coefficients for these type pairs.

Funcfl files in the *potentials* directory of the LAMMPS distribution have an ".eam" suffix. A DYNAMO single-element *funcfl* file is formatted as follows:

- line 1: comment (ignored)
- line 2: atomic number, mass, lattice constant, lattice type (e.g. FCC)
- line 3: Nrho, drho, Nr, dr, cutoff

On line 2, all values but the mass are ignored by LAMMPS. The mass is in mass units, e.g. mass number or grams/mole for metal units. The cubic

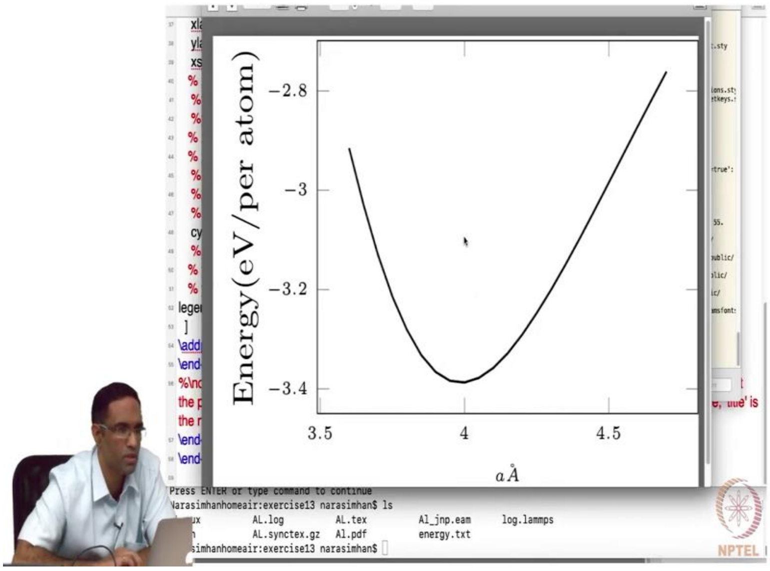
```
 -1.1283378135413557e+01 -1.1400962348393875e+01 -1.1518485462374429e+01 -1.1635947735075661e+01 -1.1753349435
543555e+01
```



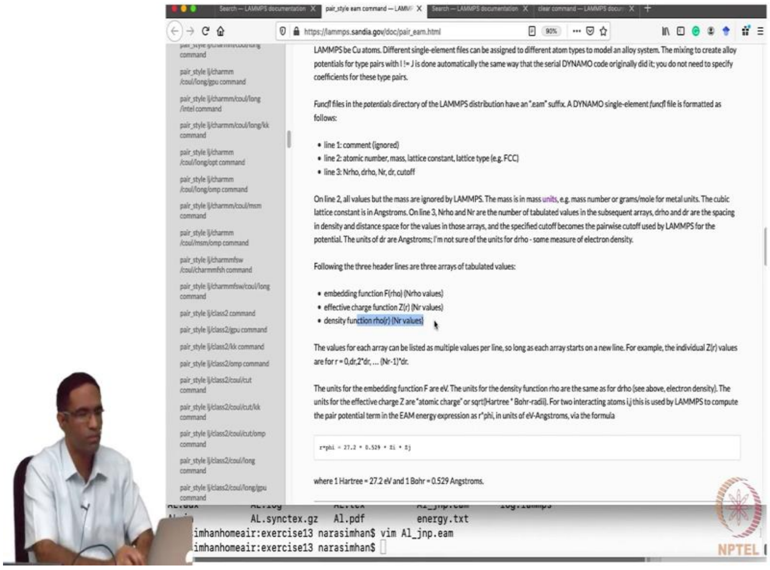
```
atom_style      atomic
boundary        p p p

# cubic diamond unit cell
variable a index 3.6 3.65 3.7 3.75 3.8 3.85 3.9 3.95 4.0 4.05 4.1 4.15 4.2 4.25 4.3 4.35 4.4 4.45 4.5 4.55 4.6
 4.65 4.7
lattice fcc ${a}
region          myreg block     0 10 &
                                0 10 &
                                0 10
#Lattice units is used, which is the  default
##in the argon example, we used box units.
create_box      1 myreg
create_atoms    1 region myreg
# Minimize  using Embedded atom method potential for Al

pair_style      eam
pair_coeff      * * Al_jnp.eam
minimize 1e-25 1e-25 100000 100000
variable latcon equal ${a}
thermo_style custom v_latcon pe
thermo 1
run 1
next a
#Go to the next a
clear
#Deletes all atoms and restores to default values
#Does not affect input script variables
jump AL.in
#Closes the current file and opens another file. In this case
#the name of this file is given so that it recalculates for a
#different value of a
~
~
~
```



```
Press ENTER or type command to continue
Narasimhanhomeair:exercise13 narasimhan$ ls
  ux          AL.log          AL.tex          Al_jnp.eam      log.lammps
  h           AL.synctex.gz   Al.pdf          energy.txt
 simhanhomeair:exercise13 narasimhan$ 
```



LAMMPS be Cu atoms. Different single-element files can be assigned to different atom types to model an alloy system. The mixing to create alloy potentials for type pairs with I != J is done automatically the same way that the serial DYNAMO code originally did it; you do not need to specify coefficients for these type pairs.

Funcfl files in the *potentials* directory of the LAMMPS distribution have an ".eam" suffix. A DYNAMO single-element *funcfl* file is formatted as follows:

- line 1: comment (ignored)
- line 2: atomic number, mass, lattice constant, lattice type (e.g. FCC)
- line 3: Nrho, drho, Nr, dr, cutoff

On line 2, all values but the mass are ignored by LAMMPS. The mass is in mass units, e.g. mass number or grams/mole for metal units. The cubic lattice constant is in Angstroms. On line 3, Nrho and Nr are the number of tabulated values in the subsequent arrays, drho and dr are the spacing in density and distance space for the values in those arrays, and the specified cutoff becomes the pairwise cutoff used by LAMMPS for the potential. The units of dr are Angstroms; I'm not sure of the units for drho - some measure of electron density.

Following the three header lines are three arrays of tabulated values:

- embedding function F(rho) (Nrho values)
- effective charge function Z(r) (Nr values)
- density function rho(r) (Nr values)

The values for each array can be listed as multiple values per line, so long as each array starts on a new line. For example, the individual Z(r) values are for r = 0,dr,2*dr, ... (Nr-1)*dr.

The units for the embedding function F are eV. The units for the density function rho are the same as for drho (see above, electron density). The units for the effective charge Z are "atomic charge" or sqrt(Hartree * Bohr-radii). For two interacting atoms i,j this is used by LAMMPS to compute the pair potential term in the EAM energy expression as r*phi, in units of eV-Angstroms, via the formula

```
r*phi = 27.2 * 0.529 * Zi * Zj
```

where 1 Hartree = 27.2 eV and 1 Bohr = 0.529 Angstroms.

```
              AL.synctex.gz   Al.pdf          energy.txt
 imhanhomeair:exercise13 narasimhan$ vim Al_jnp.eam
 imhanhomeair:exercise13 narasimhan$ 
```

And in LAMMPS, the interatomic potential for these systems are actually given in the form of a table, it is huge table. There are different formats in which embedded atom method, potential files can be given and this is one of the formats that LAAMPS can understand and use. So, I will open the file. So, for the style eam, a potential file must be assigned to each I, I pair of item types by using one or more pair coefficient commands with a single argument, which is basically the file name.

So, when you look at the input file, I have done exactly the same thing that I did with silicon here, where I just want to find out the energy versus Lattice constant curve. So, I have a variable index and so on and so forth, let us not. The only, the only difference is that I just construct an fcc Lattice and the only thing that I had to give here is a dollar a. Basically, the lattice parameter. And another thing that I want you to notice is that, here I had given the region in the default units, which is Lattice units, not units box, the Lattice units. Because, if it is units box then I have to every time calculate what my box size is.

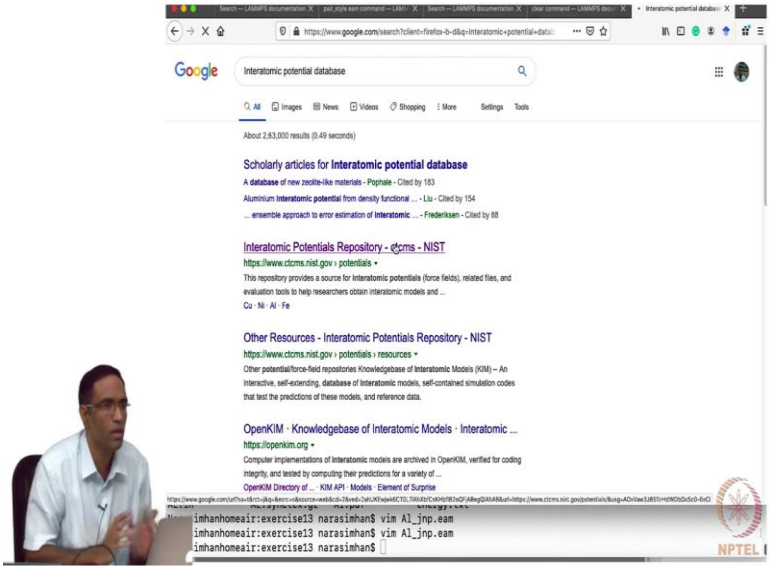
When I say, Lattice units, it is just going to be automatically taking 10 times the unit cells in each of the directions. So, I give star star and then call the corresponding file which is there in the same folder called Al underscore jnp dot eam. Perform minimization and everything like what I did for this silicon file. And if you run it, you are going to get the energy variation, but it is a good idea to look at the, let us look at the, so, you get something that looks like this, when you plot the energy versus Lattice constant. The first thing that you notice is that the Lattice constant is somewhat a little bit less than 4.

If you open up the, the potential file, the first line in the potential fi is basically a comment and it is not used anywhere. The second line basically gives you atomic number, atomic mass, the Lattice constant that was obtained from this potential and the crystal structure that is used. And then you have one another line which tells you, how the function, it is a tabulated value of the function f of rho, for various values of rho and the function, another function z of r, for various values of r. It is basically the part of the 2-body potential phi.

So, if you take a look at this, it says that there are 500 entries for f of rho. So, there should be 500 entries starting from here, so going like this. So, if you go 1,2,3,4,5 and so on, until, until somewhere here. So, there will be, there will be exactly 500 entries and then another 500 entries for the, the value of the function and then the corresponding values of, let me take a look at the file, the density function rho, rho of r. The density function rho of r, how rho varies with r, the effective charge function, how that varies with r and the embedding function f of rho, how it varies with rho.

And how rho and r are split is there in this information, d rho and d r contains that information, which is d rho, how the density is split and how the distance is actually split. So, that is the embedded atom potential and most of the time you will be able to obtain these embedded atom potentials for, for which, for whichever ones it exists.

(Refer Slide Time: 33:21)



Interatomic potential database

About 2,63,000 results (0.49 seconds)

Scholarly articles for **Interatomic potential database**

A **database** of new zeolite-like materials - Pophale - Cited by 183

Aluminium **Interatomic potential** from density functional ... - Liu - Cited by 154

... ensemble approach to error estimation of **interatomic** ... - Frederiksen - Cited by 88

Interatomic Potentials Repository - ctcms - NIST

https://www.ctcms.nist.gov › potentials

This repository provides a source for **interatomic potentials** (force fields), related files, and evaluation tools to help researchers obtain interatomic models and ...

Cu · Ni · Al · Fe

Other Resources - Interatomic Potentials Repository - NIST

https://www.ctcms.nist.gov › potentials › resources

Other **potential**/force-field repositories Knowledgebase of **Interatomic** Models (KIM) – An interactive, self-extending, **database of interatomic** models, self-contained simulation codes that test the predictions of these models, and reference data.

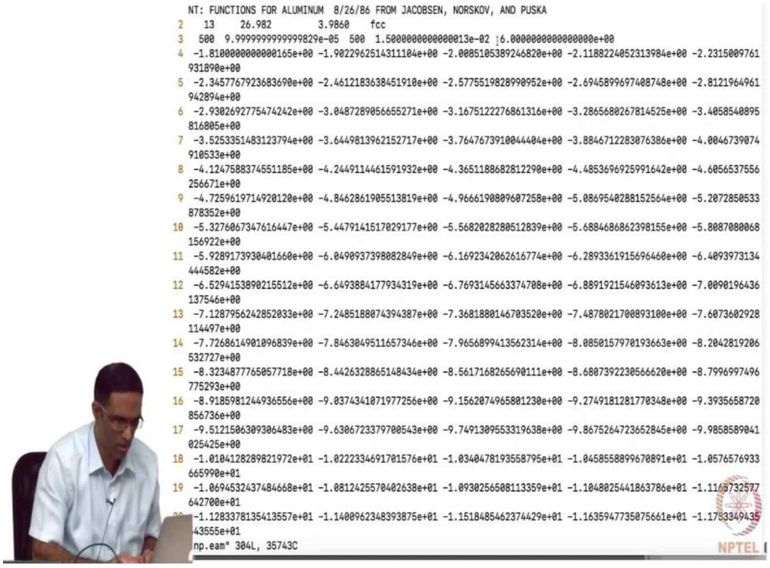
OpenKIM · Knowledgebase of Interatomic Models · Interatomic ...

https://openkim.org

Computer implementations of **interatomic** models are archived in OpenKIM, verified for coding integrity, and tested by computing their predictions for a variety of ...

OpenKIM Directory of ... · KIM API · Models · Element of Surprise

```
imhanhomeair:exercise13 narasimhan$ vim Al_jnp.eam
imhanhomeair:exercise13 narasimhan$ vim Al_jnp.eam
imhanhomeair:exercise13 narasimhan$ 
```



```
NT: FUNCTIONS FOR ALUMINUM  8/26/86 FROM JACOBSEN, NORSKOV, AND PUSKA
  13     26.982         3.9860    fcc
 500  9.9999999999999829e-05  500  1.5000000000000013e-02 6.0000000000000000e+00
-1.8100000000000165e+00 -1.9022962514311104e+00 -2.0085105389246820e+00 -2.1188224052313984e+00 -2.2315009761
931890e+00
-2.3457767923683690e+00 -2.4612183638451910e+00 -2.5775519828990952e+00 -2.6945899697408748e+00 -2.8121964961
942894e+00
-2.9302692775474242e+00 -3.0487289056655271e+00 -3.1675122276861316e+00 -3.2865680267814525e+00 -3.4058540895
816805e+00
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256671e+00
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878352e+00
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156922e+00
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444582e+00
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114497e+00
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-8.3234877765057718e+00 -8.4426328865148434e+00 -8.5617168265690111e+00 -8.6807392230566620e+00 -8.7996997496
775293e+00
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856736e+00
-9.5121506309306483e+00 -9.6306723379700543e+00 -9.7491309553319638e+00 -9.8675264723652845e+00 -9.9858589041
025425e+00
-1.0104128289821972e+01 -1.0222334691701576e+01 -1.0340478193558795e+01 -1.0458558899670891e+01 -1.0576576933
665990e+01
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642700e+01
-1.1283378135413557e+01 -1.1400962348393875e+01 -1.1518485462374429e+01 -1.1635947735075661e+01 -1.1753349435
43555e+01
np.eam" 304L, 35743C
```

```
reset_cache
    CFUNCTYPE(c_int)(lambda: None)
MemoryError
An error occurred while importing powerline module.
This could be caused by invalid sys.path setting,
or by an incompatible Python version (powerline requires
Python 2.6, 2.7 or 3.2 and later to work). Please consult
the troubleshooting section in the documentation for
possible solutions.
Error detected while processing /Users/narasimhan/.vim/bundle/powerline/powerline/bindings/vim/plugin/powerline.vi
m:
line  157:
Traceback (most recent call last):
  File "<string>", line 53, in <module>
  File "<string>", line 9, in powerline_troubleshoot
  File "/Users/narasimhan/.vim/bundle/powerline/powerline/__init__.py", line 11, in <module>
    from powerline.lib.config import ConfigLoader
  File "/Users/narasimhan/.vim/bundle/powerline/powerline/lib/config.py", line 11, in <module>
    from powerline.lib.threaded import MultiRunnedThread
  File "/Users/narasimhan/.vim/bundle/powerline/powerline/lib/threaded.py", line 7, in <module>
    from powerline.lib.monotonic import monotonic
  File "/Users/narasimhan/.vim/bundle/powerline/powerline/lib/monotonic.py", line 19, in <module>
    import ctypes
  File "/System/Library/Frameworks/Python.framework/Versions/2.7/lib/python2.7/ctypes/__init__.py", line 555, in <
module>
    _reset_cache()
  File "/System/Library/Frameworks/Python.framework/Versions/2.7/lib/python2.7/ctypes/__init__.py", line 279, in _
reset_cache
    CFUNCTYPE(c_int)(lambda: None)
MemoryError
Press ENTER or type command to continue
Narasimhanhomeair:exercise13 narasimhan$ ls
AL.aux          AL.log          AL.tex          Al_jnp.eam      log.lammps
AL.in           AL.synctex.gz   Al.pdf          energy.txt
Narasimhanhomeair:exercise13 narasimhan$ vim Al_jnp.eam
     imhanhomeair:exercise13 narasimhan$ vim Al_jnp.eam
     imhanhomeair:exercise13 narasimhan$ vim Al_jnp.eam
     imhanhomeair:exercise13 narasimhan$ ex
```

Usually it can be a hard time to find for arbitrary alloys and you should, what is the name of that, yeah NIST, Interatomic Potential Repository basically contains all possible interatomic potentials that might be there, unless new ones are invented and they have not yet been up updated, you will find most of the information in this website. So, you can take a look at this and get all the information of the potentials for which you have the interatomic (potential), elements for which the interatomic potentials basically existed.

Student: Number?

Professor: Yeah.

Student: In the precious cases, we did not mentioned atomic number, in this case why is it necessary?

Professor: It is probably used by the interatomic potential somewhere. I do not really know how the interatomic potential has actually been developed. So, it is possible that it is going to get used somewhere in the interatomic potential functional form, which is inside the, which is inside LAMMPS.

Student: And in case of Lennard-Jones, we were writing pair style, nj slash cut and the cut off length.

Professor: Correct, i j epsilon, sigma and then the corresponding cut-off radius, yeah.

Student: So, in case of eam, we do not need any cut off distance to…

Professor: It is there it is there actually. It is right, you do not have to explicitly specify it, it is there in the file, this is the cut-off.

Student: So we do not have to specify it in pair style?

Professor: Yeah you do not have to specify in pair style for the eam potential. So, now you can imagine, we plotted the variation of energy with Lattice constant. So, this amounts to plotting the variation of energy with volume as well, because a cube is nothing but the volume. So, which means you should be able to find out approximately the bulk modulus of the material.

If you just plotted this energy for various volumes then dou e by dou v, 1 by v times dou v by dou v should actually give you the bulk modulus of the material at low temperatures and for material, at low temperatures, for because, and for metals and ceramics, for really low temperatures, like close to 300 or 400 Kel, until, unless you are like close to its melting point for extremely, for temperatures far away from the melting point, the bulk modulus and the Young's modulus, the mechanical properties of the system are not significantly affected by temperature. So, you can get a rough estimate of these mechanical properties also by making a plot of this energy versus the volume. So, I think that that you should be able to do.