



LAMMPS Workshop

data file

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Atom definition

- `creat_atom`
 - `read_restart`
 - `read_data`
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What Is Data File Structure?

read_data *filename*

data file structure:

- First 2 lines are ignored.
- Lines starting with # are comments.
- Blank lines will be skipped.
- Data file has a HEADER and a BODY parts.
- The BODY of the file has some sections.
- Order of sections is *not* important!

HEADER Keywords

- *atoms*= # of atoms in system
- *bonds*= # of bonds in system
- *angles*= # of angles in system
- *dihedrals*= # of dihedrals in system
- *impropers*= # of impropers in system
- ✓ *atom types*= # of atom types in system
- ✓ *bond types*= # of bond types in system
- ✓ *angle types*= # of angle types in system
- ✓ *dihedral types*= # of dihedral types in system
- ✓ *improper types*= # of improper types in system

HEADER Keywords

- ❖ *xlo xhi= simulation box boundaries in x dimension*
- ❖ *ylo yhi= simulation box boundaries in y dimension*
- ❖ *zlo zhi= simulation box boundaries in z dimension*
- ❖ *xy xz yz= simulation box tilt factors for triclinic domain*



SECTION Keywords

- **Atom Property Sections:**

Atoms, Velocities, Masses, Shapes, Dipoles

- **Molecular Topology Sections:**

Bonds, Angles, Dihedrals, Improper

- **Force Field Sections:**

Pair , Bond, Angle, Dihedral and Improper Coefficients

- **Class 2 Force Field Sections:**

BondBond, BondAngle, MiddleBondTorsion,
EndBondTorsion, AngleTorsion, AngleAngleTorsion,
BondBond13 and AngleAngle Coefficients



Data File Example (HEADER part):

LAMMPS Description (1st line of file)

100 atoms (this must be the 3rd line, 1st 2 lines are ignored)

95 bonds (# of bonds to be simulated)

50 angles

30 dihedrals

20 impropers

5 atom types (# of nonbond atom types)

10 bond types (# of bond types = sets of bond coefficients)

18 angle types

20 dihedral types

2 improper types



Data File Example (HEADER part):

-0.5 0.5 xlo xhi

-0.5 0.5 ylo yhi

-0.5 0.5 zlo zhi (do not include this line for 2-d simulations)

Data File Example (BODY part):

Atoms

1 molecule-tag atom-type q x y z

...

N molecule-tag atom-type q x y z (N = # of atoms)

Arguments depend on atom_style!

angle	atom-ID molecule-ID atom-type x y z
atomic	atom-ID atom-type x y z
bond	atom-ID molecule-ID atom-type x y z
charge	atom-ID atom-type q x y z
dipole	atom-ID atom-type q x y z mux muy muz
dpd	atom-ID atom-type x y z
ellipsoid	atom-ID atom-type x y z quatw quati quatj quatk
full	atom-ID molecule-ID atom-type q x y z
granular	atom-ID atom-type diameter density x y z
molecular	atom-ID molecule-ID atom-type x y z
peri	atom-ID atom-type volume density x y z
hybrid	atom-ID atom-type x y z sub-style1 sub-style2 ...

Data File Example (BODY part):

Velocities

| vx vy vz

...

N vx vy vz (N = # of atoms)

Masses

| mass

...

N mass (N = # of atom types)

Data File Example (BODY part):

Bonds

1 bond-type atom-1 atom-2

...

N bond-type atom-1 atom-2 (N = # of bonds)

Angles

1 angle-type atom-1 atom-2 atom-3 (atom-2 is the center atom in angle)

...

N angle-type atom-1 atom-2 atom-3 (N = # of angles)

Dihedrals

1 dihedral-type atom-1 atom-2 atom-3 atom-4 (atoms 2-3 form central bond)

...

N dihedral-type atom-1 atom-2 atom-3 atom-4 (N = # of dihedrals)

Data File Example (BODY part):

Pair Coeffs

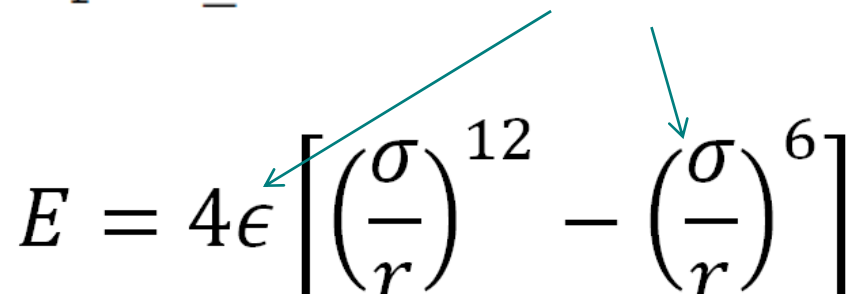
1 coeff1 coeff2 ...

...

N coeff1 coeff2 ... (N = # of atom types)

Arguments depend on pair_style!

```
pair_style lj/cut 2.5  
pair_coeff * * 1 1
```

$$E = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right]$$


Data File Example (BODY part):

Bond Coeffs


1 coeff1 coeff2 ...

...

N coeff1 coeff2 ... (N = # of bond types)

Arguments depend on bond_style!

```
bond_style harmonic  
bond_coeff 5 80.0 1.2
```


$$E = K(r - r_0)^2$$

Data File Example (BODY part):

Angle Coeffs

| coeff1 coeff2 ...

...

N coeff1 coeff2 ... (N = # of angle types)

Dihedral Coeffs

| coeff1 coeff2 ...

...

N coeff1 coeff2 ... (N = # of dihedral types)

Improper Coeffs

| coeff1 coeff2 ...

...

N coeff1 coeff2 ... (N = # of improper types)

Example of .data file

Position data for Argon atoms in a box

```
20      atoms
1       atom types

-12     12     xlo     xhi
-12     12     ylo     yhi
-12     12     zlo     zhi
```

Masses

```
1       39.95
```

Atoms

```
1       1       -10.2 -10.2 -10.2
2       1       -6.8  -10.2 -10.2
```



References

- <http://lammps.sandia.gov/doc/Manual.html>
- http://migale.jouy.inra.fr/modmol/LAMMPS_short_manual.pdf

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- Thank you for your attention.
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