readlammpsdata

Release 1.0.9

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May 12, 2024

CONTENTS:

CHAPTER

ONE

QUICK START

1.1 Installation

- PyPi install

```
pip install readlammpsdata
```

- Github install

```
git clone git@github.com:eastsheng/readlammpsdata.git
cd readlammpsdata
pip install .
```

1.2 Tests

- print version

```
import readlammpsdata as rlt
print(print_version())

"""
--------------------------------------------------
@readlammpsdata-1.0.9
>>> A script for reading and modifying LAMMPS data!
--------------------------------------------------
"""
```

- read data

```
Atoms = read_data(lmp="PVP.lmp", data_sub_str = "Atoms")
print(Atoms)
```

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```
"""
>>> Read data Atoms successfully !

     1      1      1 -0.35160000    1.000  1.00000  0.00000
     2      1      2 0.13720000   -0.337  1.00000  0.00000
     3      1      3 -0.79220000   -1.134  1.00000  1.11526
        ...
    13      1     13 0.10870000    0.222  0.44931  2.64132
    14      1     14 0.11370000   -1.868  0.86334  4.30672
    15      1     15 0.11370000   -1.804 -0.58670  3.28942
    16      1     16 0.14040000   -3.408  1.94658  2.77089
    17      1     17 0.14040000   -3.873  0.22675  2.53818
"""

Masses = read_data(lmp="PVP.lmp", data_sub_str = "Masses")
PairCoeffs = read_data(lmp="PVP.lmp", data_sub_str = "Pair Coeffs")
Bonds = read_data(lmp="PVP.lmp", data_sub_str = "Bonds")
```

CHAPTER

TWO

USAGES

2.1 General commands

CHAPTER

THREE

EXAMPLES

3.1 Read trems of lammpsdata

```
import readlammpsdata as rld
lmp ="PVP.lmp"
trems = rld.read_terms(lmp)
print(trems)
"""output
['Masses', 'Pair Coeffs', 'Bond Coeffs', 'Angle Coeffs', 'Dihedral Coeffs', 'Improper␣
↪Coeffs', 'Atoms # full', 'Bonds', 'Angles', 'Dihedrals', 'Impropers']
"""
```

3.2 Read data

- Read “Atoms”

```
Atoms = rld.read_data(lmp,"Atoms")
# or Atoms = rld.read_data(lmp,"Atoms # full")
print(Atoms)
"""output
>>> Read data Atoms successfully !

     1      1      1 -0.35160000    1.000  1.00000  0.00000
     2      1      2 0.13720000   -0.337  1.00000  0.00000
     3      1      3 -0.79220000   -1.134  1.00000  1.11526
        ...
    13      1     13 0.10870000    0.222  0.44931  2.64132
    14      1     14 0.11370000   -1.868  0.86334  4.30672
    15      1     15 0.11370000   -1.804 -0.58670  3.28942
    16      1     16 0.14040000   -3.408  1.94658  2.77089
```

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```
    17      1     17 0.14040000   -3.873  0.22675  2.53818
"""
```

- read "others trems" data

```
Masses = read_data(lmp, "Masses")
BondCoeffs = read_data(lmp, "Bond Coeffs")
AngleCoeffs = read_data(lmp, "Angle Coeffs")
DihedralCoeffs = read_data(lmp, "Dihedral Coeffs")
...
```

3.3 Read Box size

```
xyz = rld.read_box(lmp)
lx = xyz["xhi"]-xyz["xlo"]
ly = xyz["yhi"]-xyz["ylo"]
lz = xyz["zhi"]-xyz["zlo"]
print(xyz)
print(lx,ly,lz)
"""
{'xlo': -3.87301, 'xhi': 46.12699, 'ylo': -0.5867, 'yhi': 49.4133, 'zlo': -0.95115,
↪'zhi': 49.04885}
50.0 50.0 50.0
"""

lx = rld.read_len(lmp,"x")
ly = rld.read_len(lmp,"y")
lz = rld.read_len(lmp,"z")
print(lx,ly,lz)
"""
>>> Read data Header successfully !
>>> Read size of x direction successfully !
>>> Read data Header successfully !
>>> Read size of y direction successfully !
>>> Read data Header successfully !
>>> Read size of z direction successfully !
50.0 50.0 50.0
"""
```

3.4 Read atomic infos

- Number of atoms:

```
Natoms = rld.read_atom_info(lmp,"atoms")
print("Number of atoms is %s" %Natoms)

"""
>>> Read data Header successfully !
>>> Read data Header successfully !
Number of atoms is 17
"""
```

- Number of bonds:

```
Nbonds = rld.read_atom_info(lmp,"bonds")
print("Number of bonds is %s" %Nbonds)
"""
>>> Read data Header successfully !
>>> Read data Header successfully !
Number of bonds is 17
"""
```

- Number of angles, dihedrals, impropers, same as above

3.5 Read charges

```
charges = rld.read_charges(lmp)
print("Charges of atoms are %s" %charges)
print(round(sum(charges),6))
"""
>>> Read charges successfully !
Charges of atoms are [-0.3516  0.1372 -0.7922  0.1074 -0.2058 -0.2204  0.5562 -0.4121␣
↪ 0.1379  0.1379  0.1799  0.1087  0.1087  0.1137  0.1137  0.1404  0.1404]
-0.0
"""
```

3.6 Read volume

```
vol = rld.read_vol(lmp)
print(vol)
"""
>>> Read data Header successfully !
>>> Read size of x direction successfully !
>>> Read data Header successfully !
>>> Read size of y direction successfully !
>>> Read data Header successfully !
>>> Read size of z direction successfully !
>>> Read volume of system successfully !
125.0
"""
```

3.7 Sort lmp

```
rld.sort_lmp("PVP.lmp","PVP_sort.lmp")
```

3.8 lammpsdata to xyz

```
rld.lmp2xyz("PVP.lmp","PVP.xyz")
"""
----------------------  Program Start  ----------------------
>>> Read data Masses successfully !
>>> Convert the id masses to element list successfully !
>>> Read the id masses and element dicts successfully !
>>> Read data Atoms successfully !
>>> Convert lammps data (lmp) file to xyz file successfully !
--------------------- Run time: 0.04 s  ---------------------
"""
```

3.9 lammpsdata to lammpstrj

```
rld.lmp2lammpstrj(lmp,"PVP.lammpstrj")
"""
----------------------  Program Start  ----------------------
>>> Read data Masses successfully !
>>> Convert the id masses to element list successfully !
>>> Read the id masses and element dicts successfully !
>>> Read data Atoms successfully !
>>> Read data Header successfully !
>>> Convert lammps data (lmp) file to lammpstrj file successfully !
--------------------- Run time: 0.0 s  ---------------------
"""
```

3.10 others

- to be continued