

# How to create Lammmps input file with VMD

Chuanyu Liu\*

January 15, 2023

## 1 Implement with command lines

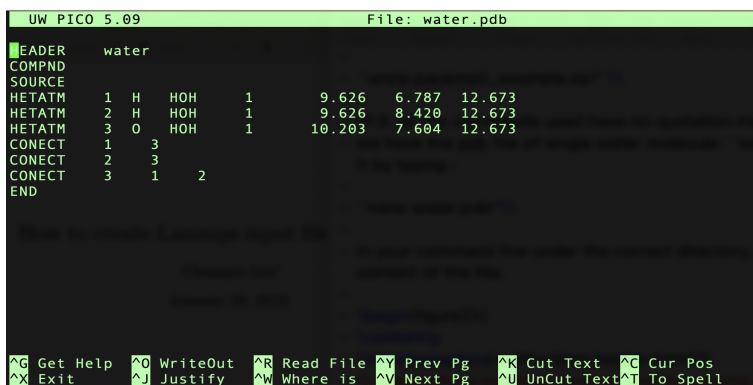
Firstly, direct to the directory “packmol”, and unzip the file by typing:

```
unzip packmol_example.zip
```

we have the pdb file of single water molecule: “water.pdb”. Let’s open it by typing :

```
nano water.pdb
```

in your command line under the correct directory, then you can see the content of the file:



```
UW PICO 5.09 File: water.pdb
HEADER      water
COMPND
SOURCE
HETATM      1  H   HOH      1      9.626   6.787  12.673
HETATM      2  H   HOH      1      9.626   8.420  12.673
HETATM      3  O   HOH      1     10.203   7.604  12.673
CONNECT      1      3
CONNECT      2      3
CONNECT      3      1      2
END
```

Figure 1. water.pdb.

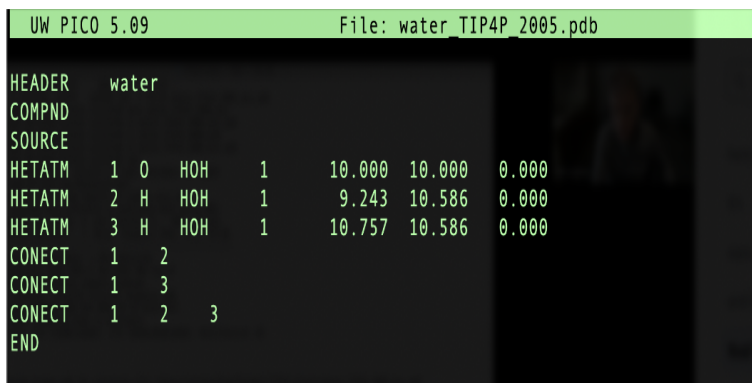
In this pdb file, there are 3 connect lines, connect lines with 2 numbers are bonds, connect lines with 3 numbers are angles that give you angular potential, but there is no

---

\*Email: wenxuan0119@uchicago.edu

charges. This file contains only one water molecule, but we are not going to use this file. Instead, we use another single water molecule file “water\_TIP4P\_2005.pdb”. Let’s have a look by typing:

```
nano water_TIP4P_2005.pdb
```

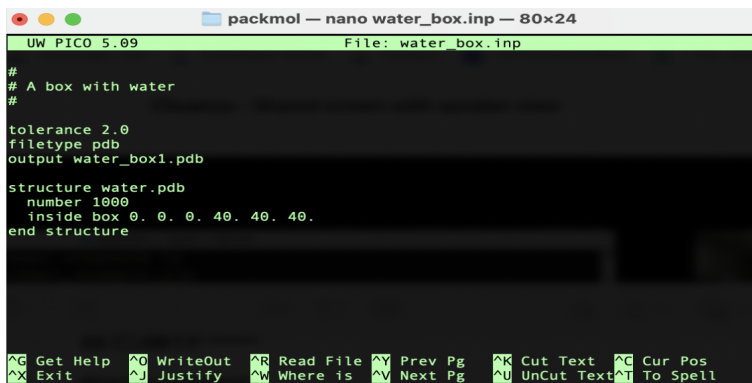


```
UW PICO 5.09 File: water_TIP4P_2005.pdb
HEADER water
COMPND
SOURCE
HETATM 1 O HOH 1 10.000 10.000 0.000
HETATM 2 H HOH 1 9.243 10.586 0.000
HETATM 3 H HOH 1 10.757 10.586 0.000
CONNECT 1 2
CONNECT 1 3
CONNECT 1 2 3
END
```

Figure 2. water\_TIP4P\_2005.pdb.

Please copy the file “water\_TIP4P\_2005.pdb” in your “packmol” directory. Then, there is another file “water\_box.inp”, you can check the file by typing:

```
nano water_box.inp
```



```
packmol — nano water_box.inp — 80x24
UW PICO 5.09 File: water_box.inp
#
# A box with water
#
tolerance 2.0
filetype pdb
output water_box1.pdb

structure water.pdb
  number 1000
  inside box 0. 0. 0. 40. 40. 40.
end structure
```

Figure 3. water\_box.inp.

In this file, you can edit it. For example, the output file name, the structure(single water molecule) you use, the number of molecule in the box, and the box size according to

the real density.

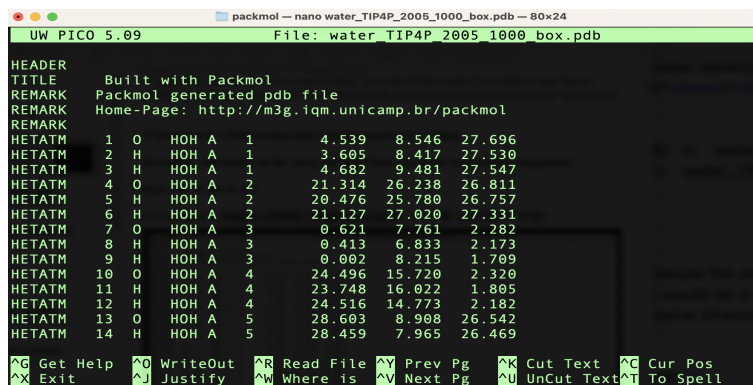
Here, we are going to simulate a system contains 1000 water molecules at 4.0 °C with “water\_TIP4P\_2005.pdb”, so the water density is nearly  $1.0g/cm^3$ , and the box size is  $31 \times 31 \times 31$ , approximately.

Then, we change the name “water.pdb” to “water\_TIP4P\_2005.pdb”, change the name “water\_box.pdb” to “water\_TIP4P\_2005\_box.pdb”, and run the command:

```
./packmol < water_box.inp
```

Packmol will read the single water molecule file and create a new file contains 1000 water molecules. There would be a new file “water\_TIP4P\_2005\_box.pdb” created in the same directory. Let’s check the file by typing:

```
nano water_TIP4P_2005_1000_box.pdb
```



```

UW PICO 5.09 File: water_TIP4P_2005_1000_box.pdb
HEADER
TITLE      Built with Packmol
REMARK     Packmol generated pdb file
REMARK     Home-Page: http://m3g.iqm.unicamp.br/packmol
REMARK
HETATM    1 O  HOH A  1      4.539   8.546  27.696
HETATM    2 H  HOH A  1      3.685   8.417  27.539
HETATM    3 H  HOH A  1      4.682   9.481  27.547
HETATM    4 O  HOH A  2     21.314  26.238  26.811
HETATM    5 H  HOH A  2     20.476  25.780  26.757
HETATM    6 H  HOH A  2     21.127  27.020  27.331
HETATM    7 O  HOH A  3      0.621   7.761   2.282
HETATM    8 H  HOH A  3      0.413   6.833   2.173
HETATM    9 H  HOH A  3      0.002   8.215   1.709
HETATM   10 O  HOH A  4     24.496  15.720   2.320
HETATM   11 H  HOH A  4     23.748  16.022   1.805
HETATM   12 H  HOH A  4     24.516  14.773   2.182
HETATM   13 O  HOH A  5     28.603   8.908  26.542
HETATM   14 H  HOH A  5     28.459   7.965  26.469
^G Get Help ^O WriteOut ^R Read File ^V Prev Pg ^K Cut Text ^C Cur Pos
^X Exit     ^J Justify  ^W Where is ^N Next Pg ^U UnCut Text ^T To Spell

```

Figure 4. water\_TIP4P\_2005\_1000\_box.pdb.

Packmol throws away all connect bonds, there is no such lines like 1 2, 1 3, to tell us which atom connects to each other, it only keeps 1000 connect angles. Besides, there is no information about the box size. Then, let’s move on with VMD. Please find the correct version of VMD to install in your own computer:

VMD\_Mac Intel

VMD\_Mac M1

VMD\_Windows

After installation successfully, click the VMD application and load the file “water\_TIP4P\_2005\_1000\_box.pdb” you created just now:

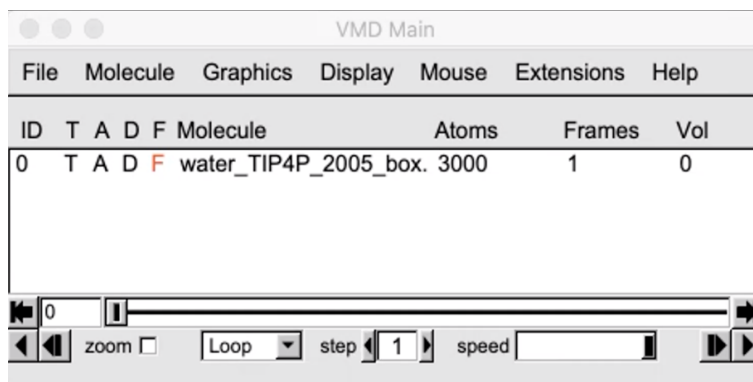


Figure 5. VMD.

After loading successfully, interface windows(see your terminal) has some new information:

```
vmd >
vmd >
vmd >
vmd >
vmd > 2023-01-19 01:08:21.439 VMD[16099:592954] TSM AdjustCapsLockLEDForKeyTrans
itionHandling - _ISSetPhysicalKeyboardCapsLockLED Inhibit
Info) Using plugin pdb for structure file /Users/jaymini/Desktop/packmol/water_T
IP4P_2005_1000_box.pdb
Info) Using plugin pdb for coordinates from file /Users/jaymini/Desktop/packmol/
water_TIP4P_2005_1000_box.pdb
Info) Determining bond structure from distance search ...
Info) Eliminating bonds duplicated from existing structure...
Info) Analyzing structure ...
Info) Atoms: 3000
Info) Bonds: 2000
Info) Angles: 0 Dihedrals: 0 Improper: 0 Cross-terms: 0
Info) Bondtypes: 0 Angletypes: 0 Dihedraltypes: 0 Improptypes: 0
Info) Residues: 1000
Info) Waters: 1000
Info) Segments: 1
Info) Fragments: 1000 Protein: 0 Nucleic: 0
Info) Finished with coordinate file /Users/jaymini/Desktop/packmol/water_TIP4P_2
005_1000_box.pdb.
```

Figure 6. VMD windows information after loading.

It shows that there are 3,000 atoms, because that’s what it reads, and it says there are 2,000 bonds. Please remember that “water\_TIP4P\_2005.pdb” file contains all information, but “water\_TIP4P\_2005\_1000\_box.pdb” file only contains the angle information: 1 2 3 , 4 5 6... no bonds information such as 1 2, 1 3... There are no bond lines in the Pdb file created by packmol.

but when we load the file “water\_TIP4P\_2005\_1000\_box.pdb”, the VMD windows show the number of bonds: 2000. It guessed the bonds! However, the angle is 0, angles are

completely ignored by VMD.

```

Info) Using plugin pdb for structure file /Users/luijten/Prog/Packmol/TIP4P_Create/water_TIP4P_2005_box.pdb
Using plugin pdb for coordinates from file /Users/luijten/Prog/Packmol/TIP4P_Create/water_TIP4P_2005_box.pdb
Determining bond structure from distance search ...
Eliminating bonds duplicated from existing structure...
Analyzing structure ...
  Atoms: 3000
  Bonds: 2000
  Angles: 0 Dihedrals: 0 Improper: 0 Cross-terms: 0
  Bondtypes: 0 Angletypes: 0 Dihedraltypes: 0 Impropertypes: 0
  Residues: 1000
  Waters: 1000
  Segments: 1
  Fragments: 1000 Protein: 0 Nucleic: 0
Finished with coordinate file /Users/luijten/Prog/Packmol/TIP4P_Create/water_TIP4P_2005_box.pdb.

```

Figure 7. VMD windows information.

Since VMD tried to guess these bonds, but we are not completely sure that this will always be correct. later we will write a Python script to check it automatically.

Actually, there are three types of potential in water molecule: the first O-H length, the second O-H length, and the angle. Instead of a water molecule. If there is a molecule like polymer or protein. There is another potential that is related to four atoms: dihedral potential. Atom 1 and atom 4 can be in different plane, because of rotation of bond.

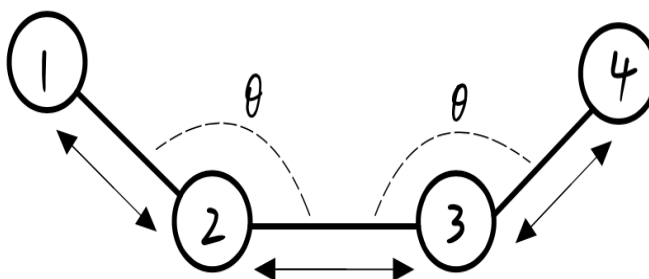


Figure 8. Dihedral potential.

Let's continue with some commands in VMD. Please typing these commands as follow:

```

: topo retypebonds
: topo guessangles
: top guessdihedrals

```

```

vmd > topo retypebonds
Info) =====
Info) Please cite TopoTools as:
Info) Axel Kohlmeyer & Josh Vermaas, (2019). TopoTools: Release 1.8
Info) https://doi.org/10.5281/zenodo.598373
Info) =====
0
vmd > topo guessangles
vmd > topo guessdihedrals
vmd > set sel1 [atomselect top "name O"]
atomselect3
vmd >

```

Figure 9. VMD windows information.

The charges in the water model is dipole moment, and the dipole moment of water depends on the distance between the oxygen and the hydrogen. It depends on the electronegativity. Water molecules are neutral, so the total charge is 0.

In Tip4p potential model, we can give the negative charge on Oxygen site instead of M site. It says, tell me the charge on the oxygen, and I will shift it to the inside when I do the simulation. Hence, in the file, you can put a negative charge simply on the oxygen site. Please type the commands:

```

set sel1 atomselect top "name O"
$sel1 set charge -1.1128
set sel2 atomselect top "name H"
$sel2 set charge 0.5564

```

```

0
vmd > topo guessangles
vmd > topo guessdihedrals
vmd > set sel1 [atomselect top "name O"]
atomselect3
vmd > $sel1 set charge -1.1128
vmd > set sel2 [atomselect top "name H"]
atomselect4
vmd > $sel2 set charge 0.5564
vmd >

```

Figure 10. VMD windows information.

And then, exit.

```
0
vmd > topo guessangles
vmd > topo guessdihedrals
vmd > set sel1 [atomselect top "name O"]
atomselect3
vmd > $sel1 set charge -1.1128
vmd > set sel2 [atomselect top "name H"]
atomselect4
vmd > $sel2 set charge 0.5564
vmd > ^Z
[1]+  Stopped                  /Applications/VMD/ 1.9.4a51-x86_64-Rev9.app/Contents/Resources/VMD.app/Contents/MacOS/VMD
dhcp-10-105-165-70:TIP4P_Create luijten$ vi water_TIP4P_2005_box.pdb
```

Figure 11. VMD windows information.

Let's set the box size by typing:  
 pbc set 31 31 31 90 90 90  
 topo writelammpsdata XXX.data full

Finally, exit from VMD, and check the file "XXX.data":

nano XXX.data

```
LAMMPS data file. CGCM style. atom_style full generated by VMD/TopoTools v1.8 on Sat Jan 07 12:50:44 CST 2023
3000 atoms
2800 bonds
1000 angles
0 dihedrals
0 impropers
2 atom types
1 bond types
1 angle types
0 dihedral types
0 improper types
-0.077000 39.923000 xlo xhi
0.047000 40.047000 ylo yhi
-0.138499 39.861501 zlo zhi

# Pair Coeffs
#
# 1 H
# 2 O

# Bond Coeffs
#
# 1 H-O

# Angle Coeffs
#
# 1 H-O-H

Masses
1 1.008000 # H
2 15.999000 # O

Atoms # full
1 1 2 -1.112800 15.640000 34.667999 39.642099 # O HOH
2 1 1 0.556400 15.841000 34.073001 39.685999 # H HOH
3 1 1 0.556400 19.371000 35.148998 39.949001 # H HOH
```

Figure 12. Input file for Lammmps created by VMD.

There are 3000 lines of all the atoms positions:

First column: atom number

Second column: water molecules number

Third column: atom types

Fourth column: charge

Fifth-seventh column: coordinates of atoms

For the size of the box, it has a tiny shift, and the reason is that in Packmol was creating molecules, and the molecules was sticking a little bit through the boundary, and it didn't want to break that. So it didn't put him on the other side. It's shifted in a little bit.

But at this moment we don't know if it didn't make mistakes. The number of bones is correct. I have not tested whether they all come in the right order, it could be wrong as we discussed above.

```

2993 998 1 0.556400 22.115000 23.850000 16.575000 # H HOH
2994 998 1 0.556400 23.479000 24.062000 16.249001 # H HOH
2995 999 2 -1.112000 0.797000 0.808000 35.848000 # O HOH
2996 999 1 0.556400 1.271000 4.408000 35.285002 # H HOH
2997 999 1 0.556400 -0.015000 5.255000 35.404999 # H HOH
2998 1000 2 -1.112000 24.296000 35.072000 10.124000 # O HOH
2999 1000 1 0.556400 25.146999 33.771999 18.504000 # H HOH
3000 1000 1 0.556400 24.028999 32.796001 18.088001 # H HOH

Bonds
1 1 2
2 1 3
3 1 4 5
4 1 4 6
5 1 7 8
6 1 7 9
7 1 10 11
8 1 10 12
9 1 13 14
10 1 13 15
11 1 16 17
12 1 16 18
13 1 19 20
14 1 19 21
15 1 22 23
16 1 22 24
17 1 25 26
18 1 25 27
19 1 28 29
20 1 28 30
21 1 31 32
22 1 31 33
23 1 34 35
24 1 34 36
25 1 37 38
26 1 37 39
27 1 40 41

```

Figure 13. Input file for Lammmps created by VMD.

```

1970 1 2953 2955
1971 1 2956 2957
1972 1 2956 2958
1973 1 2959 2960
1974 1 2959 2961
1975 1 2962 2963
1976 1 2962 2964
1977 1 2965 2966
1978 1 2965 2967
1979 1 2968 2969
1980 1 2968 2970
1981 1 2971 2972
1982 1 2971 2973
1983 1 2974 2975
1984 1 2974 2976
1985 1 2977 2978
1986 1 2977 2979
1987 1 2980 2981
1988 1 2980 2982
1989 1 2983 2984
1990 1 2983 2985
1991 1 2986 2987
1992 1 2986 2988
1993 1 2989 2990
1994 1 2989 2991
1995 1 2992 2993
1996 1 2992 2994
1997 1 2995 2996
1998 1 2995 2997
1999 1 2998 2999
2000 1 2998 3000

Angles
1 1 2 1 3
2 1 5 4 6
3 1 8 7 9
4 1 11 10 12

```

Figure 14. Input file for Lammmps created by VMD.