How to create Lammps input file with VMD

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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:

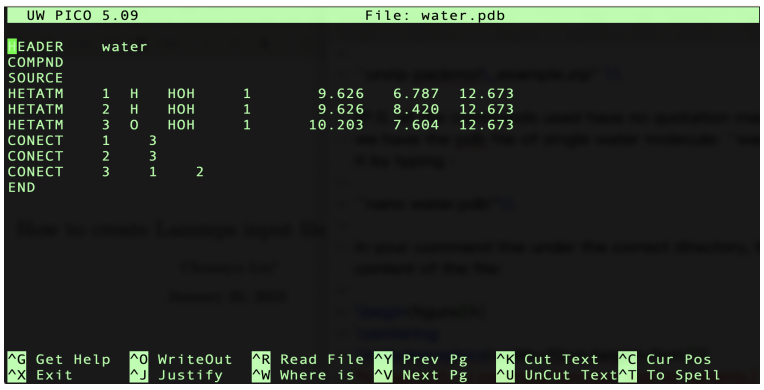

Figure 1. water.pdb.

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

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charges. This file contains only one dater 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

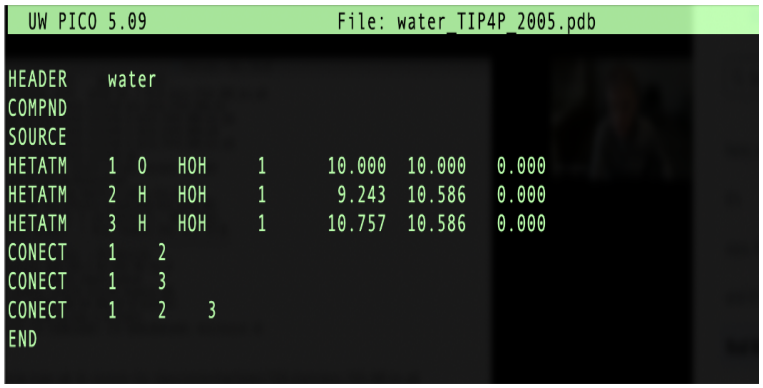

Figure 2. water_TIP4P_2005.pdb.

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

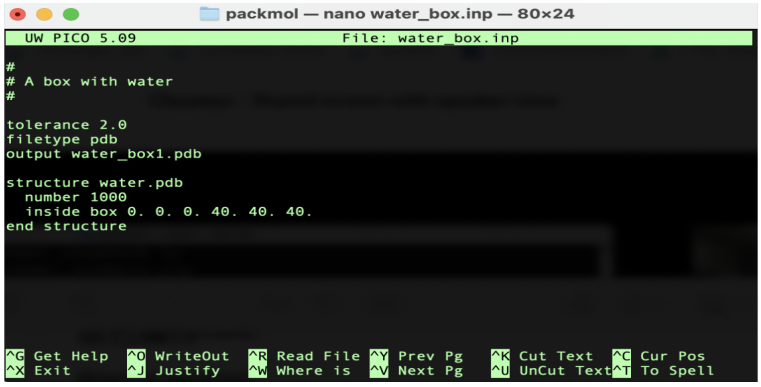

Figure 3. water_box.inp.

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 $1.0 g/cm^3$, and the box size is 31×31×31, 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

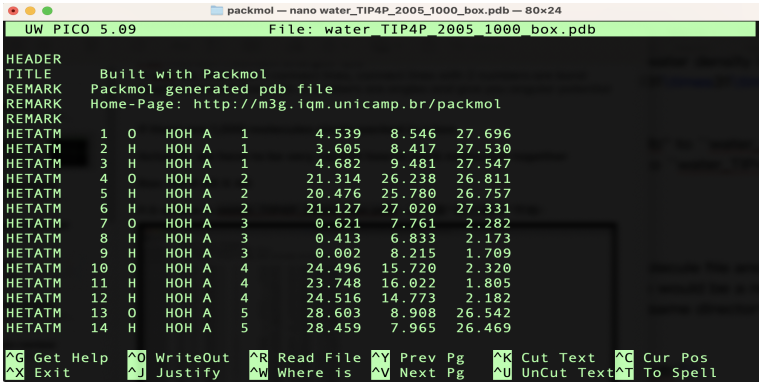

Figure 4. water_TIP4P_2005_1000_box.pdb.

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:

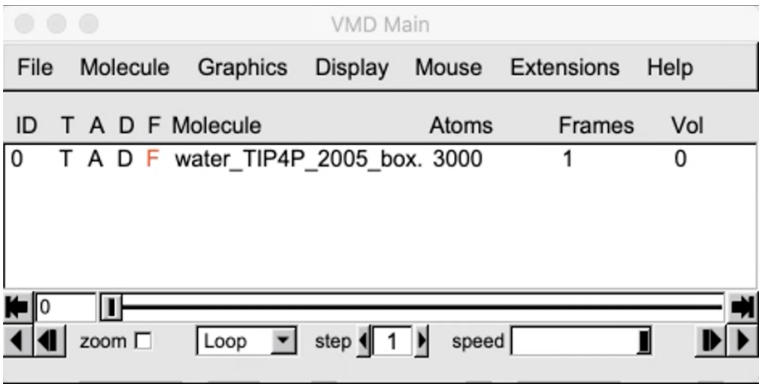

Figure 5. VMD.

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

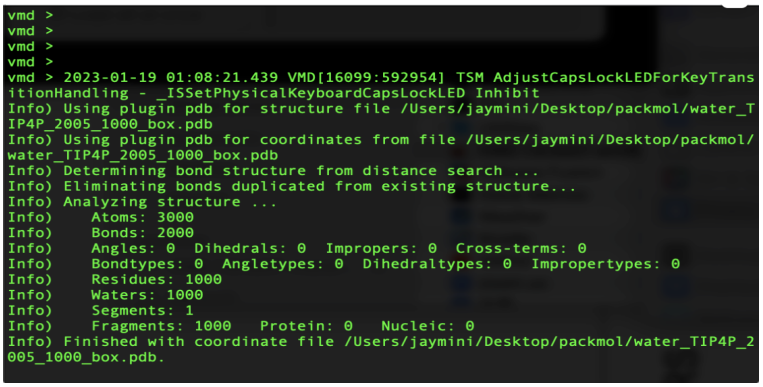

Figure 6. VMD windows information after loading.

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  Impropers: 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.

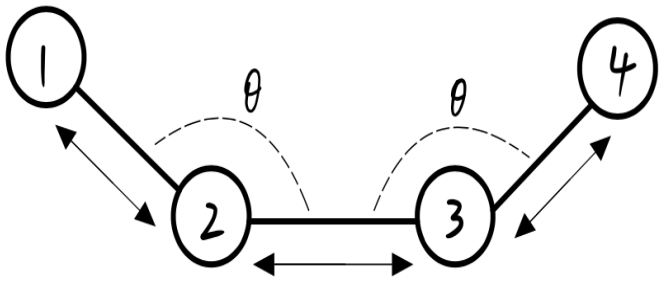

Figure 8. Dihedral potential.

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

: topo retypebonds
: topo guessangles
: top guessdihedrals

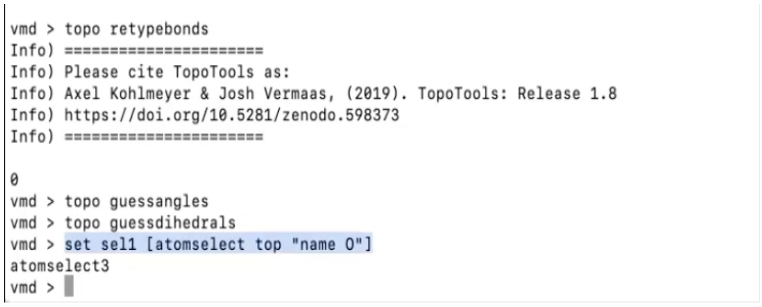

Figure 9. VMD windows information.

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 0”
$sel1 set charge -1.1128
set sel2 atomselect top “name H”
$sel2 set charge 0.5564

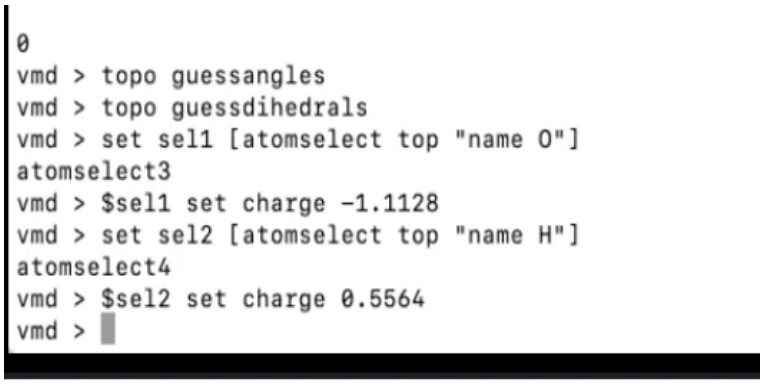

Figure 10. VMD windows information.

And then, exit.

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

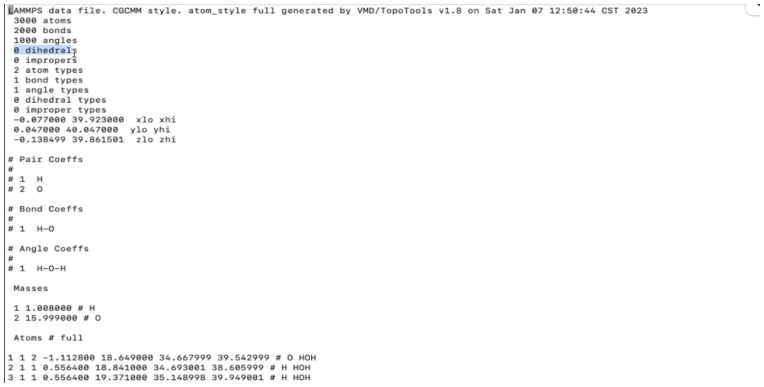

Figure 12. Input file for Lammps created by VMD.

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.

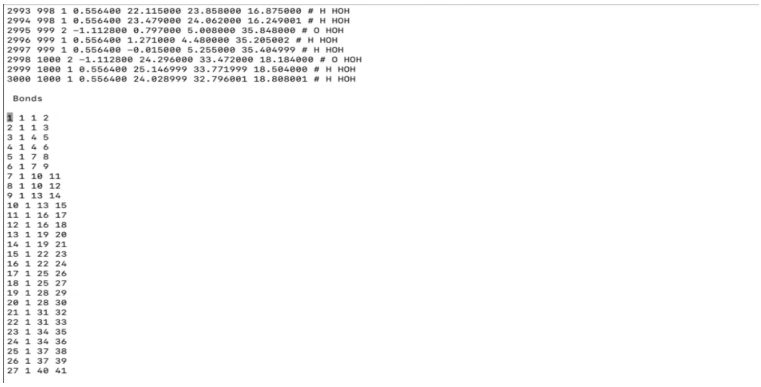

Figure 13. Input file for Lammps created by VMD.

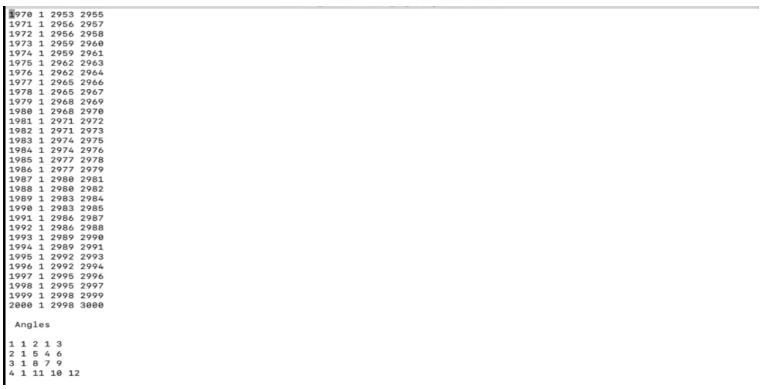

Figure 14. Input file for Lammps created by VMD.