GROMACS Tutorial 2 - One methane in water

In this tutorial I'll show you how to create a system containing one OPLS methane in a box of TIP4PEW water.

Setup

As before, we need a structure file, a topology file, and parameter files. We're going to use the GROMACS tool *gmx pdb2gmx* to generate the topology from a pdb file.

Setup residues for pdb2gmx

For this molecule we'll be using the OPLS force field. The force field is located in the top-level force field directory (probably `/usr/share/gromacs/top` or something similar).

If you're unsure where your GROMACS installation is do:

```
$ echo $GMXPREFIX
```

If you are properly sourcing the GROMACS configuration file, this will give you the installation location. Look for the directory `share/gromacs/top` in that directory and go into it (*e.g.*, if GMXPREFIX is `/usr` then go to `/usr/share/gromacs/top`). Or you can simply go to `$GMXDATA/top` .

Let's take a look at the force field directory's its contents:

```
$ cd oplsaa.ff
$ ls
```

You'll see several files, but we're only interested in a few of them for now. Notice `forcefield.itp` . This is the main file used in simulations. Inside you'll see a `[ defaults ]` section as well as the inclusion of two other files - one for bonded interactions and one for non-bonded interactions. We're also interested in `atomtypes.atp` which gives the descriptions for the cryptic `opls_####` terms as well as the `aminoacids.rtp` which give a list of recognized residues used for the *gmx pdb2gmx* command.

Open `atomtypes.atp` with your text editor. The following opens it with `vim` :

```
$ vim atomtypes.atp
```

Go to the line with `opls_138` . Notice the comment says `alkane CH4` , so we are on the right track here for our methane. However, notice the mass in the second column - this is only the carbon for a CH4 group, so we also need the hydrogens. This is an "all atom" model - every atom is represented. The corresponding hydrogen is `opls_140` . You'll probably also want to look at the supporting info of the OPLS force field paper (http://pubs.acs.org/doi/suppl/10.1021/ja9621760/suppl_file/ja11225.pdf). The parameters in the paper should match up with the parameters that we'll look at in a minute. Now make a note of these two atom types and close the file.

Let's take a look at `ffnonbonded.itp` for these two atom types:

```
$ grep opls_138 ffnonbonded.itp
$ grep opls_140 ffnonbonded.itp
```

Here we see the name of the atom type, the bond type, the mass, the charge, ptype, sigma, and epsilon. Make a note of the charge for each one - we'll need it for our new residue. As a side note, `ffbonded.itp` will use the bond type for the bond types, angle types, and dihedral types.

Before continuing, you may want to copy your top-level force field directory directory somewhere, like your home directory, since we'll be modifying it and adding some files. To copy it to your home directory do:

```
$ cp -r $GMXDATA/top $HOME/GMXLIB
```

You might have to be root to do it. Now change the `$GMXLIB` environmental variable to:

```
$ export GMXLIB=$HOME/GMXLIB
```

Add the above to your `.bash_profile` to make it permanent. Now do:

```
$ cd $GMXLIB
```

You are now in the copy of the director you made, and all simulations will use that directory instead of the one provided in the GROMACS default directory.

Now go into `oplsaa.ff` and open `aminoacids.rtp`. You'll notice several residues already in the file. We're going to add a new file called `methane.rtp` for our methane with a residue that we'll call `CH4`. Close `aminoacids.rtp`. We'll need to tell *gmx pdb2gmx* the atoms and bonds in the atom in our residue file. We could also tell it the angles, but we'll leave them out, since *gmx pdb2gmx* will figure it out for us. You should create with the following contents and save as `methane.rtp` in the `oplsaa.ff` directory:

```
[ bondedtypes ]
; bonds  angles  dihedrals  impropers all_dihedrals nrexcl HH14 RemoveDih
  1      1       3          1         1             3      1    0

; Methane
[ CH4 ]
 [ atoms ]
   C      opls_138    -0.240     1
   H1     opls_140     0.060     1
   H2     opls_140     0.060     1
   H3     opls_140     0.060     1
   H4     opls_140     0.060     1
 [ bonds ]
   C      H1
   C      H2
   C      H3
   C      H4
```

A few notes on the above file: the `[ bondedtypes ]` comes from `aminoacids.rtp` and is required. Under `[ atoms ]` you can name them anything you want, as long as they match the pdb file we are going to create later. Notice in the first column we gave the atom names, then we gave the atom types, the charges, and then the charge group. Under `[ bonds ]` we just tell it how each atom is connected to the others. In this case, `C` has a connection to each hydrogen. We could optionally add `[ angles ]`, but as stated earlier, GROMACS will sort this out for us. Now close the file. See section 5.6 for more information about this.

Create pdb file and run *gmx pdb2gmx*

Now we are ready to create the pdb file. There are several programs out there to create molecule structure files. Avogadro (http://avogadro.cc/wiki/Main_Page) is one of those. An alternative to this is to use "xleap" from the AmberTools (http://ambermd.org/#AmberTools) package. In Avogadro simply click any spot in the window and you'll get a methane. Save this file as `methane.pdb`. Your file should look something like this. Save this somewhere in your home directory but not anywhere in `$GMXLIB`.

Change `LIG` to `CH4` everywhere in `methane.pdb`. Also change the first `H` to `H1`, the second to `H2` and so on. PDB files are fixed format, so keep the beginning of each column in the same place. The CONNECT and MASTER records also will not be needed, so they can be removed. Also go ahead and change `UNNAMED` to `METHANE`. Your modified file should look something like this:

```
COMPND    METHANE
AUTHOR    GENERATED BY OPEN BABEL 2.3.2
HETATM    1  C   CH4     1      -0.370   0.900   0.000  1.00  0.00           C
HETATM    2  H1  CH4     1       0.700   0.900   0.000  1.00  0.00           H
HETATM    3  H2  CH4     1      -0.727   0.122   0.643  1.00  0.00           H
HETATM    4  H3  CH4     1      -0.727   0.731  -0.995  1.00  0.00           H
HETATM    5  H4  CH4     1      -0.727   1.845   0.351  1.00  0.00           H
END
```

Save the file as `methane.pdb`.

Now we can use *gmx pdb2gmx* to create GROMACS .conf and .top files:

```
$ gmx pdb2gmx -f methane.pdb
```

You'll be prompted to choose a force field. Choose OPLS. If you have an option between two different force field directories, choose the OPLS that is in the copied directory you made. For the water model choose TIP4PEW. If you get an error that GROMACS cannot find residue `CH4` you may be using the wrong force field.

Three files will be created: `conf.gro`, `posre.itp`, and `topol.top`. `conf.gro` is our file containing just one methane, topol.top is the system's topology file, and posre.itp is the optional position restraint file for our solute (methane). We won't be using that one. In the `topol.top` file notice that there is an `[ angles ]` section as promised. You'll also want to rename the compound in `topol.top`. Take a look and explore each file. Chapter 5 of the GROMACS manual will help you understand the topology file more.

Note: `topol.top` *and* `methane.pdb` *will be used again in other tutorials.*

For those who use *gmx pdb2gmx* to generate topologies for large proteins, things can get more complicated. This is merely a simple example, and really we probably could have found this topology somewhere else.

Solvate system

Our structure file and topology file only have our methane thus far. We need to add waters by using *gmx solvate*:

```
$ gmx solvate -cp conf.gro -o conf.gro -cs tip4p -p topol.top -box 2.3 2.3 2.3
```

Parameter files

We'll be using the same files **`from the previous tutorial`** (../../../_downloads/f13ec2618761f5a2efb7bba9efd9db2e/mdp.tar.gz).

Simulation

We'll be using the same sequence as last time. This assumes your mdp files are in a directory named `mdp`:

```
$ gmx grompp -f mdp/min.mdp -o min -pp min -po min
$ gmx mdrun -deffnm min
$ gmx grompp -f mdp/min2.mdp -o min2 -pp min2 -po min2 -c min -t min
$ gmx mdrun -deffnm min2
$ gmx grompp -f mdp/eql.mdp -o eql -pp eql -po eql -c min2 -t min2
$ gmx mdrun -deffnm eql
$ gmx grompp -f mdp/eql2.mdp -o eql2 -pp eql2 -po eql2 -c eql -t eql
$ gmx mdrun -deffnm eql2
$ gmx grompp -f mdp/prd.mdp -o prd -pp prd -po prd -c eql2 -t eql2
$ gmx mdrun -deffnm prd
```

Tip: You may want to put the above commands in a bash script called `run`. Add the following lines to the top of the script:

```
#!/bin/bash

set -e
```

Then do:

```
$ chmod +x run
```

To run the script do:

```
$ ./run
```

Your script should look **`like this`** (../../../_downloads/f879faf468157d9bfe5060dcfcabfe5d/run). `set -e` tells bash to stop the script if there is an error.

Analysis

Let's calculate something called the radial distribution function (https://en.wikipedia.org/wiki/Radial_distribution_function). First, we need to create an index file:

```
$ gmx make_ndx -f conf.gro
```

```
> a C
> a OW
> q
```

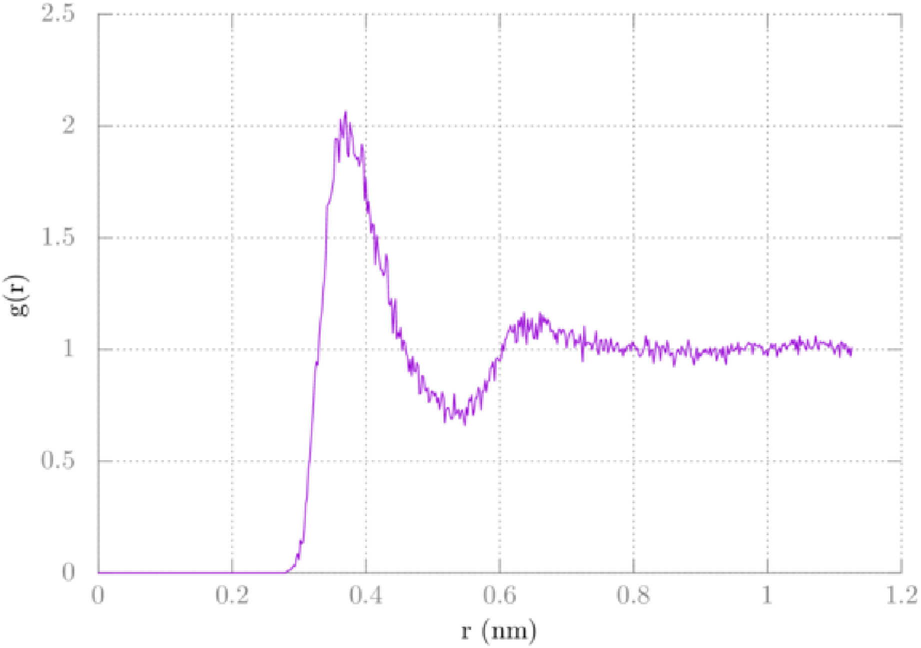
Now run *gmx rdf*:

```
$ gmx rdf -f prd.xtc -n index.ndx
```

At the prompt select `C` for the reference group. Then select `OW`. Then type `CTRL-D` to end. A plot of the result, found in columns 1 and 3 of the data would be plotted by doing the following in gnuplot:

```
> plot 'rdf.xvg' u 1:3 w l
```

It should look something like this:



C-OW RDF

Summary

In this tutorial we learned how to create a residue template file (.rtp) for use with *gmx pdb2gmx*. We created a structure for OPLS methane and the generated a topology for it. From there we put water around it using *gmx solvated*. After this we ran a simulation, just like last time. Lastly, we found the C-OW radial distribution function using *gmx rdf*.

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