CHM 579 LAB 3B(I): MOLECULAR DYNAMICS SIMULATION OF SOLVATED ACETONE

The goal of this lab is to become more comfortable with running simulations in GROMACS and to learn how to create your own input files for basic simulations. The system of study is a single acetone molecule $(CH_3)_2CO$ solvated in SPC/E water. The lab procedure *assumes independent work* with GROMACS manual. Refer to Lab 2b for general information about running GROMACS.

The GROMACS manual website:
http://manual.gromacs.org/current/

GROMACS tutorials website:
http://www.gromacs.org/Documentation/Tutorials

Scholar's User Guide:
https://www.rcac.purdue.edu/compute/scholar/guide/

Lab Procedure

We will use the acetone model from the paper "Kirkwood-Buff derived force field for mixtures of acetone and water" by S. Weerasinghe and P. E. Smith (J. Chem. Phys. 118, p 10663, 2003). This model corresponds to the *united atom* type: the methyl groups are represented by a *single interaction site*.

Step 1

From the `/scratch/carter/g/gchopra/class/CHM579/` directory on Scholar copy `lab3b_1/` to your `CHM579/` folder located in your home directory.

Step 2

Simplify the acetone model by making it rigid using constraints. Be sure to understand the molecular geometry before going to the next step. Calculate how many constraints are needed to have fully rigid acetone molecule.

Step 3

Write a topology file (`topol.top`) for a system containing only one acetone molecule and no water. Table I in the paper is useful for specifying geometry of acetone. Check the structure of the topology file from previous examples.

Look through *Chapter 5: Topologies* and read carefully *Section 5.7: File Formats* of GROMACS 5.0 manual in PDF format:
ftp://ftp.gromacs.org/pub/manual/

Find the combination rules that were used in the paper and invoke those rules in the `[default]` section, see Table II in particular.

Step 4

Create a coordinate file (`conf.gro`) for a single acetone molecule contained in a simulation box of approximately 1.8 x 1.8 x 1.8 nm^3. You don't need to have a perfect structure.

IMPORTANT: You can get the geometry of acetone from the Computational Chemistry Comparison and Benchmark Database:
http://cccbdb.nist.gov/

WARNING: The coordinate file `conf.gro` has a *fixed format*. The columns are in fixed positions. Refer to section 5.7.6

Step 5

Check that you can actually run a short simulation of this isolated acetone molecule, 10 steps are enough. Remember that to run the simulation you must load the GROMACS module first, then execute `grompp`, and finally `mdrun`. Read the output of these two programs, and *pay attention* to error and warning messages.

Step 6

Check the trajectory from the simulation with *Visual Molecular Dynamics* software and ensure that the final conformation has the proper molecular structure. VMD is a free molecular viewer.

You can check more information about VMD at:
http://www.ks.uiuc.edu/Research/vmd/

For visualization of trajectories, read the "VMD-excersices.pdf" file and the VMD class tutorial we have created for you.
VMD class tutorial - http://web.ics.purdue.edu/~gchopra/class/public/pages/VMD_tutorial/

For more details, check the official VMD tutorial:
http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/index.html

There is a local version of VMD in the iTaP's lab Windows computer. Click on the *Start* button and search for *Visual Molecular Dynamics*. When you see VMD's logo, click on it to launch the program.

Running VMD locally implies that you need to transfer the files you need to open with VMD from Scholar to your local computer.

RECOMMENDATION: If you prefer to run VMD on Scholar, you need to have an X11 terminal supported by an X-Win Server, for example Cygwin. You can launch VMD on Scholar through the X11 terminal with the following instructions:

To load the VMD module on Scholar: `module load vmd`

Once you loaded the module you can run VMD from the terminal.

To run VMD in the background (leaving the terminal open): `vmd &`

Step 7: YOUR TURN!

You may continue with the following only after steps 2 through 5 were completed successfully.

(A) Include `[moleculetype]` `SOL` for the SPC/E water model in the topology file.

GROMACS provides an *auxiliary script* `genbox` to fill the simulation box with water molecules. Check `genbox -h` and carefully read the program help and manual. Use genbox to solvate your initial simulation box that has the solitary acetone molecule.

1. Visualize your new conformation with VMD. Take a snapshot of your system.

(B) Equilibrate a system to T=300 *K* and P=1 *atm*. For that, you need to equilibration stages: a 50 *ps* of NVT, and 100 *ps* of NPT (with stochastic dynamics, `integrator=sd`).

2. Check that temperature and pressure have correct values.

After that, perform a short molecular dynamics simulation under NPT conditions, 100-200 *ps* should be enough.

3. Calculate the radial distribution function for every pair of `[atomtypes]`.

Step 8: EXTRA-CREDIT ASSIGNMENT!

(C) Include the harmonic bonds, angle, and improper dihedral in topology file. You may use information in Table 1.

Equilibrate the system and perform calculations in NPT ensemble.

I. Calculate RDFs.

II. Discuss the both simulations.

Step 9: LAB REPORT

You can report the results for either Step 7, or Steps 7 and 8.

4. Describe details of your simulations: number of molecules in simulation, temperature, pressure, cut-off distances, length and time step of simulation, etc.

5. Describe the force fields used and the interactions that are included in these force fields.

6. Describe constraints if any.

7. Plot RDFs for each pair of atom types.

8. Compare RDFs between water sites with those from the previous lab. Comment on any differences you observe.

9. Discuss shapes of acetone-water RDFs. Do they make sense to you?

10. Based on the positions of the first peaks in the water-acetone RDFs, make a hand sketch of the first water shell around the acetone molecule.