Molecular dynamics simulation of water

After studying this chapter, you will be able to carry out the

1) Calculations of radial distribution functions between oxygen atoms of two water molecules in liquid water.
2) Calculations of potentials of mean force between two oxygen atoms of two water molecules in liquid water.
3) Calculation of diffusion constant of water molecules in liquid water.

Keywords: Potential of mean force, diffusion constant, radial distribution function

Introduction

The molecular Dynamics simulation of water can be performed by using the following steps.

Generation of initial configuration:

For generating initial configuration of water, a pdb file of a single water molecule is needed.

The pdb file of a water molecule is given below. Note that the pdb file consists of the following contents.

```
HEADER    water
COMPND
SOURCE
HETATM    1  OW  SOL    1       0.000   0.000   0.000
HETATM    2  HW1 SOL    1      -0.560  -0.410  -0.750
HETATM    3  HW2 SOL    1      -0.541   0.733   0.462
CONECT    1    3
CONECT    2    3
CONECT    3    1    2
END
```

In linuxoprating system, you have already installed packmole. Then, go to the directory packmole

cd home/username/packmole

After that, make a file liquidwater.inp. the format of this is given below

****

file made by Mayank Dixit

A liquid water

#

tolerance 2.0

filetypepdb

output liquidwater.pdb

structure pwtt.pdb

number 2048

inside cube 0. 0. 0. 40.0

end structure

****

Then give the command:

./packmole<liquidwater.inp

<enter>

When job will be completed, the liquidwater.pdb file will be generated.

In this file, initial configuration of water is given.

Conversion of pdb to gro:

First of all, make a directory by giving the command

mkdirpurewater

Then copy liquidwater.pdb this file into this directory. Then, convert this file into gro format.

editconf –f liquidwater.pdb –o liquidwater.gro

<enter>

Generation of index file:

Make_ndx –f liquidwater.gro –o index.ndx

<enter>

q

<enter>

The index file has been generated.

The itp file of water molecule

****

; .itp file for SPC rigid water

[moleculetype]

; Name nrexcl

SOL 3

[atoms]

; nr type resnrresidu atom cgnr charge mass

1 OW 1 SOL OW 1 -0.8476 15.99940

2 HW 1 SOL HW1 1 0.4238 1.00800

3 HW 1 SOL HW2 1 0.4238 1.00800

[settles]

; OW functdohdhh

1 1 0.1 0.16330

```
[ exclusions ]
1    2    3
2    1    3
3    1    2
;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
```

Topology file for liquid water:

```
;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;

; prameters are taken from opls force field

[ defaults ]
;  nbfunc    comb-rule      gen-pairs     fudgeLJfudgeQQ
   1          2              yes           0.5       0.8333

[ atomtypes ]
; name     mass       charge    ptype      sigma          epsilon
   OW    15.99940     -0.8476      A      3.166e-01        0.65060
   HW    1.008000      0.4238      A      0.00000          0.00000

#include "water.itp"

[ system ]
```

liquid water

[molecules]

;mol_name number

SOL 2048

****

Now in purewater directory, you have water.itp, index.ndx, topol.top, and liquidwater.gro files.

Energy minimization of initial configuration:

The energy of system can be minimized with the help of em.mdp file. The em.mdp file is given below.

****

; em.mdp - used as input into grompp to generate em.tpr file

; Parameters describing what to do, when to stop and what to save are given below.

integrator = steep ; Algorithm (steep = steepest descent minimization)

emtol = 1000.0 ; Stop minimization when the maximum force < 1000.0 kJ/mol/nm

emstep = 0.01 ; Energy step size

nsteps = 5000 ; Maximum number of (minimization) steps to perform

; Parameters describing how to find the neighbors of each atom and how to calculate the interactions

nstlist = 1 ; Frequency to update the neighbor list and long range forces

ns_type = grid ; Method to determine neighbor list (simple, grid)

rlist = 1.0 ; Cut-off for making neighbor list (short range forces)

coulombtype = PME ; Treatment of long range electrostatic interactions

rcoulomb = 1.0 ; Short-range electrostatic cut-off

rvdw = 1.5 ; Short-range Van der Waals cut-off

pbc = xyz ; Periodic Boundary Conditions

****

Now, you have to give the following command to generate em.tpr file

grompp –f em.mdp –c liquidwater.gro –n index.ndx –p topol.top –o em.tpr

<enter>

The em.tpr file is generated

Now, give the command to run energy minimization:

mdrun –v –s em.tpr –c em.gro

When this job is completed, the final lines are:

****

Steepest Descents:

Tolerance (Fmax) = 1.00000e+03

Number of steps = 5000

Step= 0, Dmax= 1.0e-02 nm, Epot= -4.33711e+04 Fmax= 8.39995e+02, atom= 1039

writing lowest energy coordinates.

Steepest Descents converged to Fmax< 1000 in 1 steps

Potential Energy = -4.3371094e+04

Maximum force = 8.3999481e+02 on atom 1039

Norm of force = 2.4711336e+02

gcq#1: "I Live the Life They Wish They Did" (Tricky)

****

You will get em.gro file. This file will have minimum energy configuration.

Performance of Final MD of liquid water

To perform final MD the input files are em.gro, water.itp, topol.top, index.ndx, fullMD.mdp

The fullMd.mdp file is given below

****

integrator = md

dt = 0.002 ; ps

nsteps = 90000 ; = 8 ns tot

nstcomm = 1

nstxout = 0

nstvout = 0

nstfout = 0

nstlog = 9000

nstenergy = 9000

nstxtcout= 500

nstlist = 10

ns_type = grid

coulombtype = PME

rcoulomb = 1.0

vdwtype = cutoff

rvdw = 1.5

pme_order = 4

optimize_fft = yes

;Couplig Temp

tcoupl = v-rescale

tau_t = 0.1

tc-grps = System

ref_t = 298.0

;Costrain Bond

constraints = all-bonds

constraint_algorithm = LINCS

;Coupling P

Pcoupl = berendsen

Pcoupltype = isotropic

tau_p = 1

compressibility = 4.5e-5

ref_p=1

;Generate velocity

gen_vel = yes

gen_temp = 298.0

gen_seed = 173529

****

Now give the following command to generate fullMD.tpr file

grompp –f grompp.mdp –c em.gro –n index.ndx –p topol.tpr –o fullMD.tpr

<enter>

The fullMD.tpr file is generated. To perform full MD of liquid water give following command

mdrun –v –s fullMD.tpr –c fullMD.gro

<enter>

When job is completed, the following output files will be generated.

traj.xtc, fullMD.gro, traj.trr etc

Radial distribution function between oxygen-oxygen of two water molecules:

If you want to calculate g(r) between two oxygen atoms, you have to make a new index file in which you have defined the index of oxygen atoms of water molecules.

Give the following command to generate the index file of oxygen atom.

make_ndx –f fullMd.tpr –o Oxygenindex.ndx

<enter>

Type

t O (here you have write atoOm type oxygen as defined in topol.top file here it is 'O')

<enter>

q

<enter>

You can see that Oxygenindex.ndx have been generated.

Give the following command to calculate g(r) between two oxygen atoms.

g_rdf -f traj.xtc –s fullMD.tpr –n Oxygenindex.ndx –o rdfO-Owater.xvg

<enter>

Select group

Type

'OW'

<enter>

Again type

'OW'

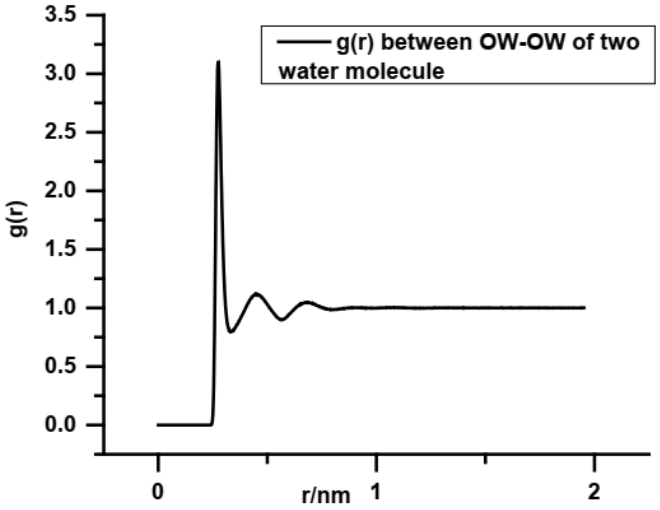
<enter>

Now you can see rdfOW-OWwater.xvg file is generated.

Note: If you want to plot acurve between r vs g(r). You have to install xmgrace in linuxopreting system. Then give following command

xmgracerdfOW-OWwater.xvg

<enter>

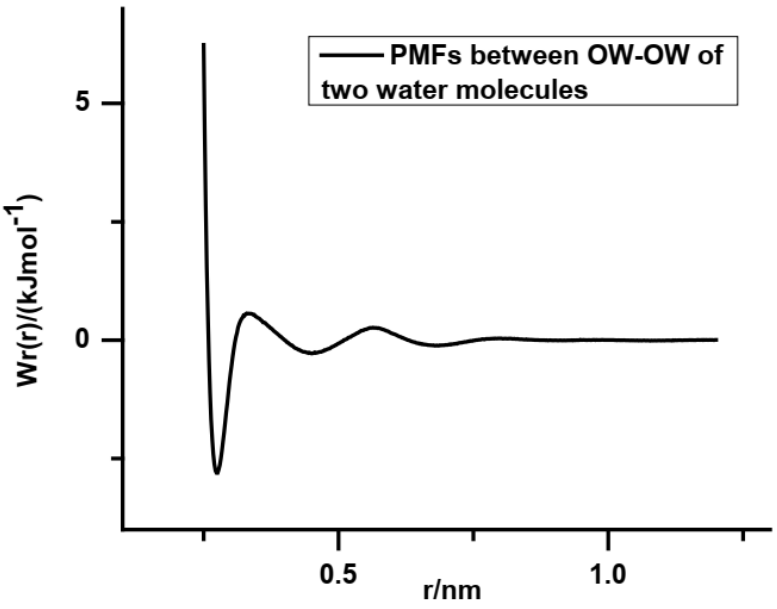


Calculation of Potentials of mean force (PMFs) between OW-OW of two water molecules:

With the help of radial distribution function (g(r)) you can calculate PMFs. The relation between PMFs and g(r) is given below

$$W(r) = -kT \ln g(r) \qquad (1)$$

W(r) is the potentials of mean force between two argon atoms, k is the Boltzmann constant, T is the temperature of system and g(r) is radial distribution function g(r) between OW-OW of two water molecules.



Calculation of diffusion coefficient of argon atom:

The diffusion constant of water molecule can be calculated as

g_msd -f traj.xtc –s fullMD.tpr –n index.ndx –o diffusionwater.xvg

<enter>

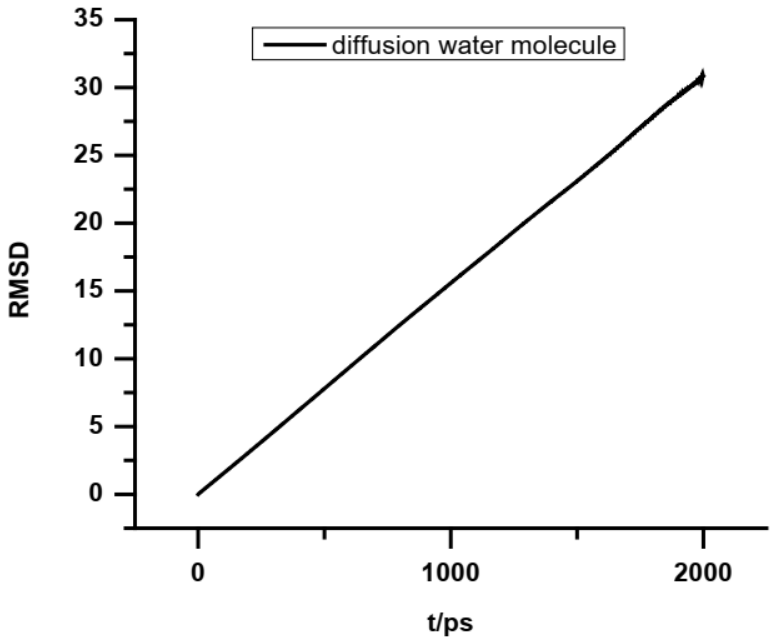
Select group

Type SOL

<enter>

When job will be completed, diffusionwater.xvg file will be generated.

Analyze this file properly. In this file, on x-axis, time in picoseconds is given and on y-axis mean square displacement of water molecule is given. If you plot a graph between rmsdand ti you will get a straight line. The slope of this straight line gives diffusion coefficient of w molecule.



Summary

In this chapter, you have been provided the algorithms tor doing the following tasks using Gromacs.

1) Calculations of radial distribution functions between oxygen atoms of two water molecules in liquid water.
2) Calculations of potentials of mean force between two oxygen atoms of two water molecules in liquid water.
3) Calculation of diffusion constant of water molecules in liquid water.

Exercise: Perform the above simulations.