Diffusion processes and properties of atomistic water models

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Computational Task: Atomistic water simulations with GROMACS

In this exercise we will simulate the properties for different water models with GROMACS which is a freely available Molecular Dynamics software package (www.gromacs.org). We will focus on the SPC, SPC/E and TIP3P water models.

C1: Running the simulation

Please download the corresponding zip-archive from the webpage. After unpacking, you will find different files in the directory.
The files are:

- spc216.gro: pre-equilibrated water structure with 216 solvent molecules
- grompp.mdp: Parameters for the simulation
- topol.top: Topology file for the water simulation which includes a link to the force field parameters
- index.ndx: File which is needed for the analysis

Open the water configuration (spc216.gro) with vmd.

```
vmd spc216.gro
```

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The file shows a pre-equilibrated water structure with 216 solvent molecules. Have also a look at the other files in the zip-archive. Copy the files into three different directories with the names spc, spce and tip3p. First we will start the simulation of the SPC water. You can either download your own copy of GROMACS or use the CIP computers. In the following, the usage of GROMACS with the CIP computers will be described.
Type the command

```
/group/allatom/gromacs-4.6.1-plumed-1.3/bin/grompp_mpi_d -v
```

The command grompp prepares the input files for the simulation. After this, the simulation can be conducted via

```
/group/allatom/gromacs-4.6.1-plumed-1.3/bin/mdrun_mpi_d -v
```

The system is simulated for 500 ps with a time step of 2 fs at 300 K.
After the simulation is finished, change into the spce or tip3p directory. Change the line

```
#include "spc.itp"
```

into

```
#include "spce.itp"
```

or

```
#include "tip3p.itp".
```

in the corresponding topol.top - file. Use the commands grompp and mdrun to perform the simulations for all three water models.

C2: Analysis of the simulation - Radial distribution function

GROMACS also offers a broad variety of analysis tools. The radial distribution function between water molecules gives a first hint towards the local water structure. To investigate the radial distribution function, use the command

```
/group/allatom/gromacs-4.6.1-plumed-1.3/bin/g_rdf_mpi_d -n index
```

and have a look at the output file with xmgrace or gnuplot. Compare the radial distribution function for all three water models and interpret the results (peaks, distance between peaks, differences between the water models ...).

C3: Analysis of the simulation - Hydrogen bond analysis

A crucial feature of water is the pronounced effect of hydrogen bonds between the oxygen and hydrogen atoms. The occurrence of these bonds is mainly reliable for many important properties of water. We can determine the number of hydrogen bonds within the simulated system via

```
/usr/local64/gromacs4.0.4-gcc4.3-static/bin/g_hbond_mpi_d -n index
```

where the results can be compared between the different water models. Please calculate the average number of hydrogen bonds for a water molecule. What is the meaning of donors and acceptors?

C3: Analysis of the simulation - Mean-square displacement

The diffusion coefficient D can be calculated via the mean-square displacement function

$$< \Delta r(t)^2 >= 6Dt \tag{1}$$

after a time t. You can calculate the mean-square displacement in GROMACS via

```
/usr/local64/gromacs4.0.4-gcc4.3-static/bin/g_msd_mpi_d -n index
```

Have a look at the output files for the different water models and compare them. What are the differences? Can you identify a linear ($< \Delta r(t)^2 > \sim t$) and a ballistic regime ($< \Delta r(t)^2 > \sim t^2$)?