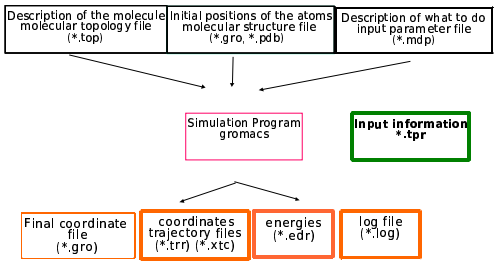
Molecular Dynamics Simulations ANALISYS

Analysis a MD simulation



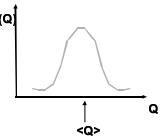
Analysis of molecular dynamics simulation

- To follow the evolution of a property Q (energy, volume, density,…) as a function of time Q(t).
- Useful to study the behavior of the system or to monitor the equilibration

Main Questions: Convergence? and Accuracy?

Analysis of molecular dynamics simulation

- Average of property Q $\langle Q \rangle = \frac{1}{N}\sum_{i=1}^{N} Q_i$
- Fluctuation of property Q $\delta Q = Q - \langle Q \rangle$
- Mean square deviation of property Q $\sigma^2 = \frac{1}{N}\sum_{i=1}^{N}\left(Q_i - \langle Q \rangle\right)^2$
- Distribution of property Q values
  - Count the number of times that a given Q value occurs (e.g. histograms)
  - Gives the probability distribution of Q: P(Q)



Analysis of MD simulations of butane in water solution at 1 atm and at 300 K and 350 K

temperature and pressure

To calculate the average values after the equilibration. use the option **-b** *time (time need to equilibrate in ps)* of g_energy

- How lang are the **temperature** and **pressure** average values after equilibration? Do they agree with your setting?

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Energy and Volume

- Report the average values of the potential energy, kinetic and total energy together with their standard deviation. Compare the average potential energy, kinetic and total energy of the MD simulation at 300 K and at 350 K
- Report the average values of the volume together with their standard deviation. Compare the average volume of the system at 300 K and 350 K

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•Report the average values of the dihedral angle C-C-C-C.

•Plot the value of the dihedral angle C-C-C-C in function of the time and its distributions for both simulations. For which value/values of the dihedral angle do you observe a maximum in the distribution function?

•Is the average value of the dihedral meaningful or meaningless?

• Compare the values observed for the dihedral angle at 300 and 350 K.

• Compare the dihedral values with the EM result.

To analyze angles and distances

Index files (*.ndx) are used to define a atom or a group of atoms with a group name. Index groups are necessary for almost every gromacs tools.
The option **-n index_file** indicates which index_file the tool has to read.

example index_file
> angle.ndx

```
[ dihedral ]    ; [ group_name ]
1 5 8 11        ; list of the atom numbers you want in the
                        group. Attention the order is important
```

Index_file can be generated: by hand
by the tool **make_ndx:**
make_ndx -f *.gro -o *.ndx
> h (for help)

To analyse the angle values:

•Create an index group in the index file with the atom's numbers refering to the dihedral C-C-C-C

•Use the tools g_angle to extract the information on the dihedral angle from the trajectory file:

Indicate to g_angle where it has to look for information
g_angle -f traj.xtc -s topol.tpr -n angle.ndx .....

Tell to g_angle what it has to do
.....-type dihedral -ov cccc.xvg -od cccc_distr.xvg

To analyse the angle values (cont)

g_angle plots the average angle of a group of angles as a function of time (using option -ov); computes the angle distribution for a number of dihedrals. (using option -od)
g_angle -f traj.xtc -s topol.tpr -n angle.ndx -type dihedral -ov cccc.xvg -od cccc_distr.xvg

•Use xmgrace to visualize the files *cccc.xvg* and *cccc_distr.xvg*

•To plot the dihedral angle values between 0-360 degree in xmgrace:
command Data > Transformation > evaluateExpression
select the set
type in the window formula y=mod(y+360,360)
click on apply

Repeat the operation how many time you need.

MD Simulation of liquid water

•Take the geometry file (water.gro) and the topology file (water.gro) together with ff.itp and ffnb.itp.

•Which non-bonded interactions do you have? And which analytical functions and parameters does the force field use?

•Create the parameter file to minimize the system.

•Run the minimization.

•Create the parameter file for around 200 ps simulation (using 2 fs time step) at the following simulation conditions:
Constant temperature (298 K) and pressure (1 atm)
Non-bonded interaction cut-off 1.2 nm

•Run the MD simulation starting from the minimized structure.

•Check that you have at least 100 ps after the equilibration if not run longer.

To be ready for next Wednesday