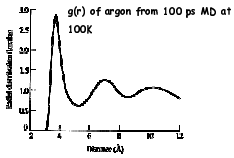
# Molecular Dynamics Simulations
# ANALISYS
# (II)

## Radial Distribution functions g(r)

- Useful to describe the structure of a system
- Gives the probability of finding an atom (or molecule) a distance r from another atom (or molecule)
- Calculated by counting the average number of atoms (or molecules) within a given distance range (r+δr - r) (bin) over the simulation and normalizing by the expected number of atoms (molecules) within the correspond volume




## Radial Distribution functions $g_{X-Y}$ (r)
## Tool: g_rdf

To calculate the radial distribution functions use the tool g_rdf

**g_rdf -f traj.xtc -s topol.tpr -n index.ndx -o rdf.xvg -cn cn.xvg**

Select a reference group and group of interested.

**index.ndx**: should contain a reference group (atoms X) and a group of interested (atoms Y). Use *make_ndx* to create the index file.

**rdf.xvg**: radial distribution function X-Y. Use xmgrace to plot it
**cn.xvg**: cumulative number

## Number of hydrogen bond
## g_hbond

To calculate number of hydrogen bond between system A and B:

**g_hbond -f traj.xtc -s topol.tpr -n index.ndx -num hbnum.xvg -ang hbang.xvg -dist hbdist.xvg**

Select a group A and group B.

**index.ndx**: should contain group A and B. Use *make_ndx* to create the index file.

**hbnum.xvg**: number of h-bond as a function of time
**hbang.xvg**: angle distribution of all hydrogen bonds
**hbdist.xvg**: distance distribution of all hydrogen bonds.

**Analysis of MD simulations of liquid water at 1 atm and at 298 K.**

•Report the density of the system and its standard deviation.

•Simulate one water molecule in vacuo (using the parameter file vacuo.mdp) and calculate the heat of vaporization of the simulated water with its standard deviation.

•Compare the results for simulated liquid water with the experimental values.

• Calculate the radial distribution function for $r_{O\,O}$ and the cumulative number.
•Calculate the number of hydrogen bonds in your system

•How many (on average) water molecules are in the first shell?
•How many h-bond for water molecules do you observed?
•How does the water model perform?

## Predict molecular properties:
## Density and Heat of vaporization

Experimental values
Density=997.1 kg/m$^3$ ΔHvap=43.9 kJ/mol at 298 K
ref:
W. Wanger and A. Pruss *J. Phys. Chem. Ref. Data* **31**, *387* (2003).

Calculated values:
???????? ????????????? at 298 K

Density = mass/volume

Heat of vaporization =
Potential energy (1 molecule in gas phase)
– Potential energy (1 molecule in liquid phase)
+R*Temperature

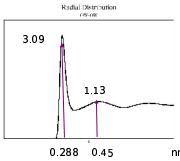
R= 8.3 J /(mol K)

g_energy: to extracts the density value and the potential energy value from the energy file after equilibration.

## Radial Distribution functions g(r) of water

From neutron diffraction:

$g(r_{OO})$




ref:
A.K. Soper, M.G. Philips,
*Chem Phys.* **107**, 47 (1987)

From MD simulations

- Create a group (using make_ndx) with all the oxygen atoms (atom name OW)
- g_rdf calculates radial distribution functions in different ways. The normal method is **around a (set of) particle(s)**, the other method is around the center of mass of a set of particles

END!!!!!!!!!!

Thank you for your attention