IX school of neutron Scattering “Francesco Paolo Ricci”

# Neutron Diffraction Experiment on Water sample

Gudrun and EPSR data analysis

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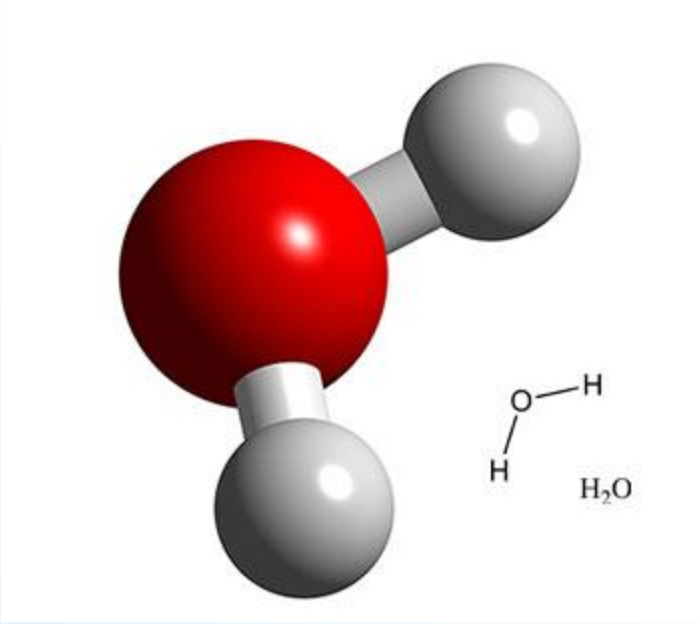
# Contents

- Sample and instrument
- Structure factors definition
- Data analysis
- Conclusions

# The sample:water

## T=45 ºC




- Neutron Diffraction experiment
- Instrument: SANDALS at ISIS neutron facility (pulsed source)

# SANDALS

**Small Angle Neutron Diffractometer for Amorphous and Liquid Samples**

**Using SANDALS it is possible to measure the static structure factor, S(Q), of a material over a wide range of momentum transfers**

| | |
|---|---|
| Incident Wavelength: | 0.05 to 4.5 Å |
| **Q-range:** | **0.1 to 50 Å** |
| Moderator: | Liquid methane at 110K |
| Incident Flight Path: | 11m |
| Final Flight Paths: | 0.75m to 4.0m |

# The neutron diffraction experiment

Total Structure Factor

Atomic concentrations and scattering lengths

$$F(Q) = \sum_{\alpha,\beta} c_\alpha c_\beta b_\alpha b_\beta (S_{\alpha\beta}(Q) - 1)$$

Partial Structure Factors

$$S_{\alpha\beta}(Q) - 1 = 4\pi\rho \int_0^\infty r^2 (g_{\alpha\beta}(r) - 1) \frac{\sin(\mathrm{Qr})}{\mathrm{Qr}} \mathrm{dr}$$

Atomic density

Partial Pair Distribution Functions

# How can we obtain $S_{\alpha\beta}(Q)$?

- We have to perform an isotopic substitution of H with D
- We have 3 $S_{\alpha\beta}(Q)$ to evaluate
- We need 3 different concentration of D:

  - $H_2O$ (0%)
  - HDO (50%)
  - $D_2O$ (100%)

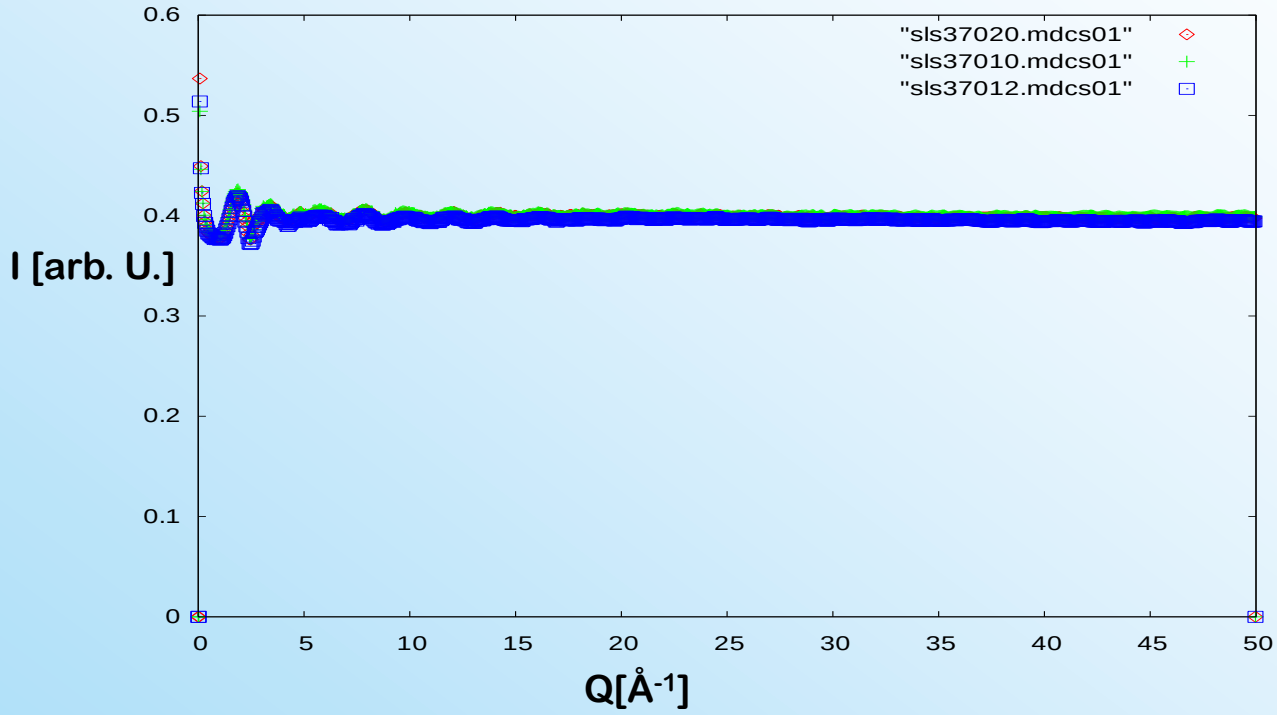
# How we can perform the data analysis?

- Can subtraction
- MC  simulation to correct the inelastic contribution
- Start with EPSR to refine the potential
- Start with accumulation
- Analysis  Results
- Conclusions

# Can Subtraction

- Can subtraction to obtain only the sample signal
- In principle each can is different although is made of the same material
- So we have to measure each of them

# Can Signals




- $H_2O$
- $D_2O$
- HDO

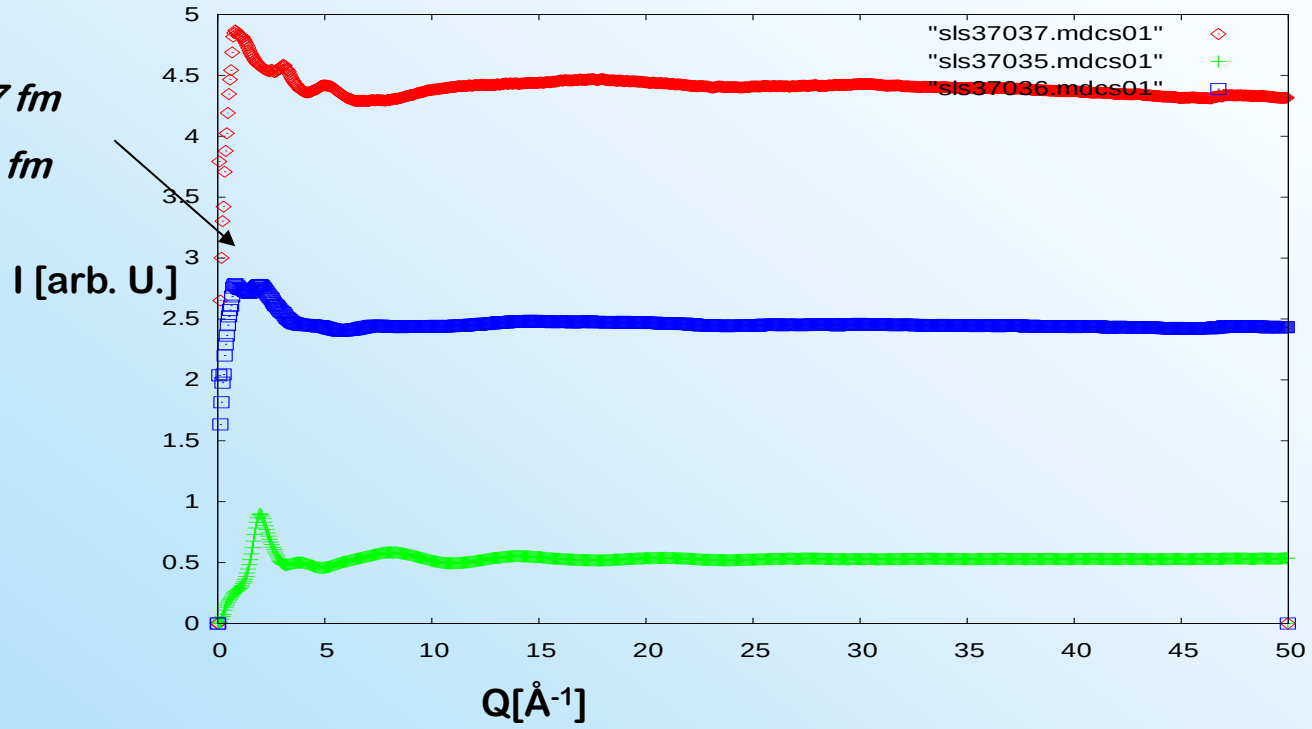
*Nominal thickness: 0.1 cm*

| Sample Can | Thickness (cm) |
|---|---|
| $H_2O$ | 0.095 |
| $D_2O$ | 0.090 |
| HDO | 0.094 |

# Inelastic Correction

$b_D$= +6.67 fm

$b_H$= -3.74 fm




- $H_2O$
- $D_2O$
- HDO

- The slope of the H2O at low q values is due to the inelastic scattering
- The $q \rightarrow \infty$ level of different sample is due to the difference between the incoherent differential cross sections of hydrogen and deuterium

# MC simulation to correct the inelastic contribution

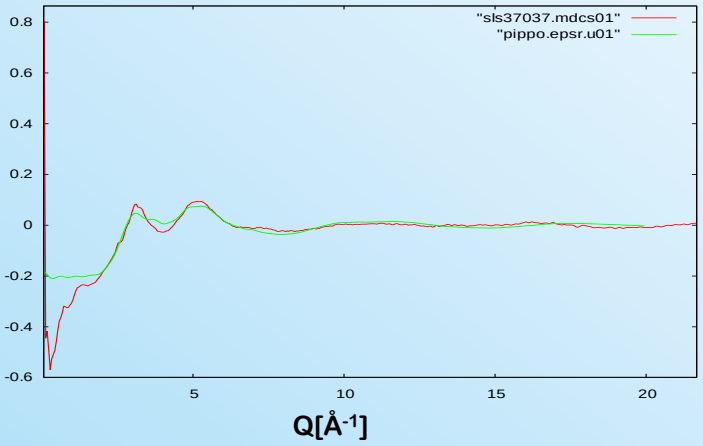
- We start an EPSR simulation without potential refinement
- We used the SPC-E (Simple Point Charge Enhanced) reference potential

$$U^{ref} = \varepsilon_{\alpha\beta}\left[\left(\frac{r_{\alpha\beta}}{\sigma_{\alpha\beta}}\right)^{6} - \left(\frac{r_{\alpha\beta}}{\sigma_{\alpha\beta}}\right)^{12}\right] + \frac{q_\alpha q_\beta}{4\pi\varepsilon_0 r_{\alpha\beta}}$$

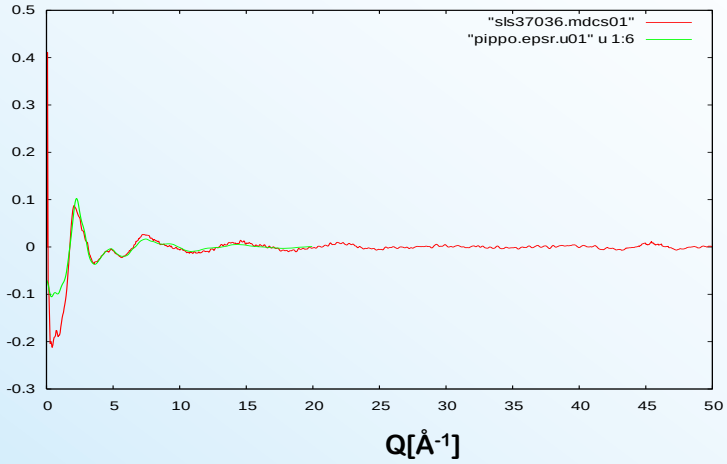
| Atom | ε (KJ/mol) | σ (Å) | q(e) |
|---|---|---|---|
| O | 0.65 | 3.166 | -0.8476 |
| H | 0 | 0 | 0.4238 |

# MC simulation to correct the inelastic contribution

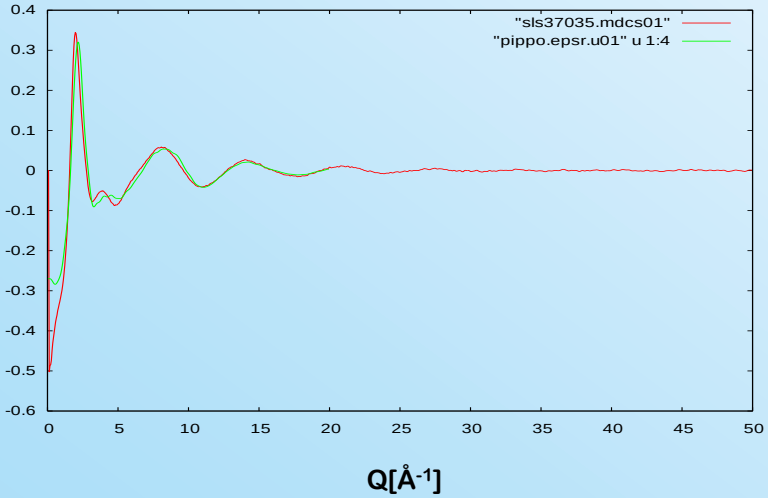
## $H_2O$



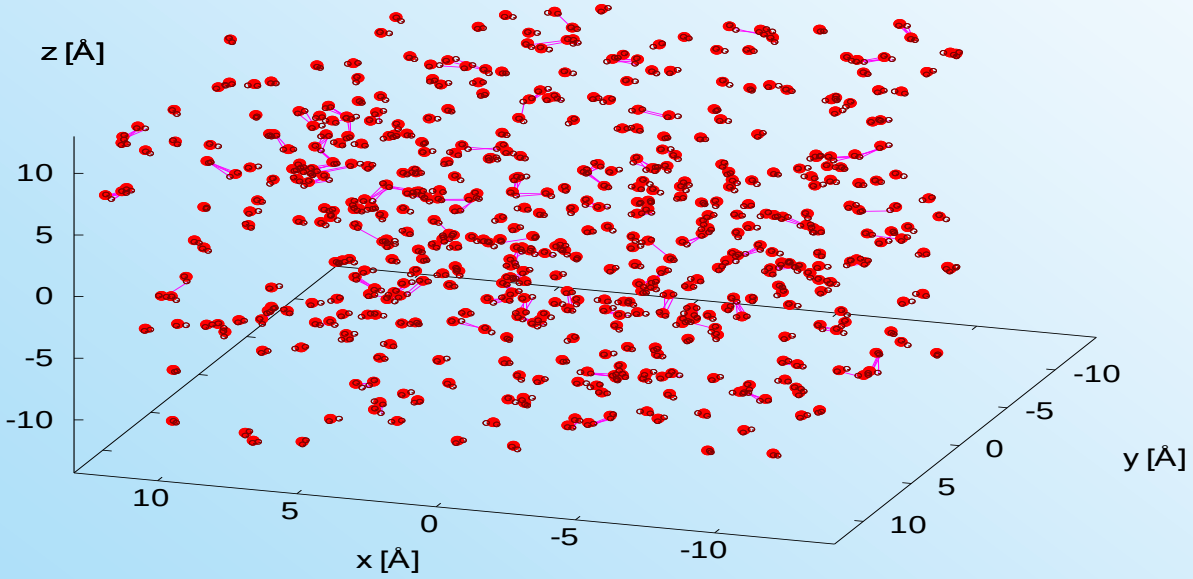

## HDO




## $D_2O$



# Start with EPSR to refine the potential

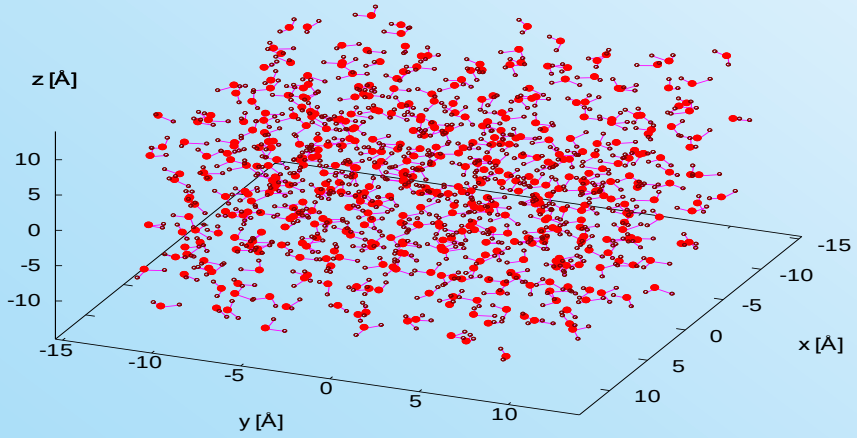



- Cubic box with 500 water molecules
- Box edge of ~25 Å

- We switched on the referential potential refinement of the system used for the MC simulation
- Wait for the system to thermalize

# Start with accumulation

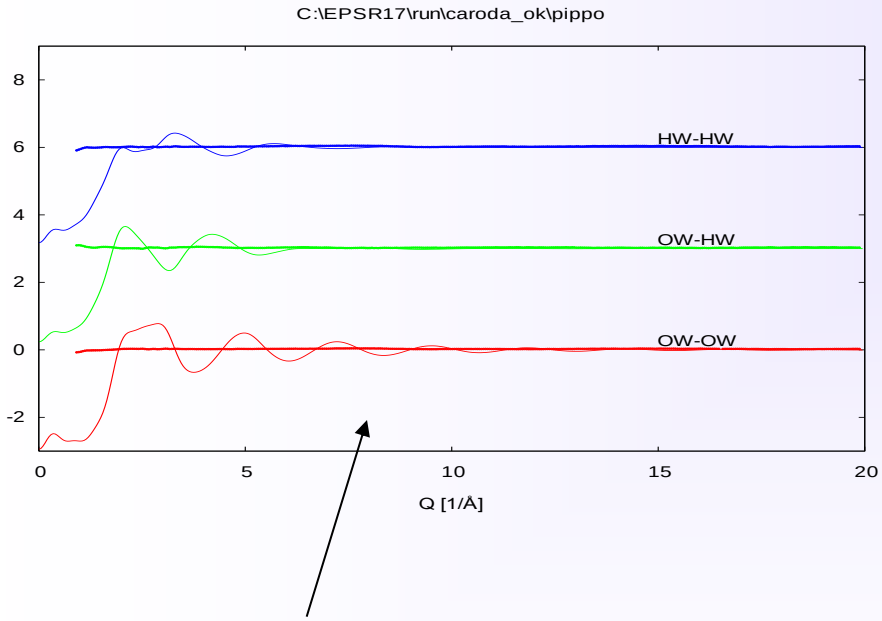
- Once the system reach the energy minimum we start accumulating configurations (put iinit=0)
- EPSR makes an average of equivalent configurations of the system




Increase of H bonds!!

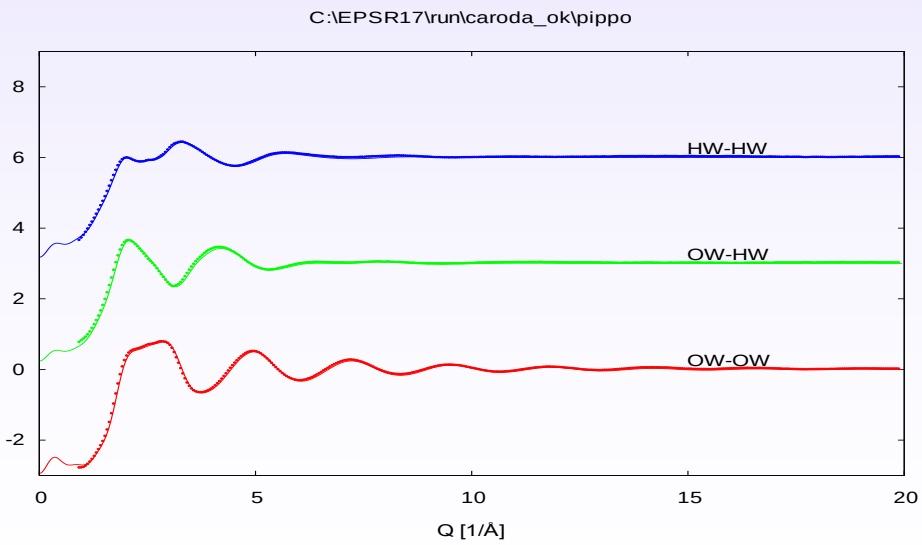
# Analysis Results

## Fit and difference with experimental data



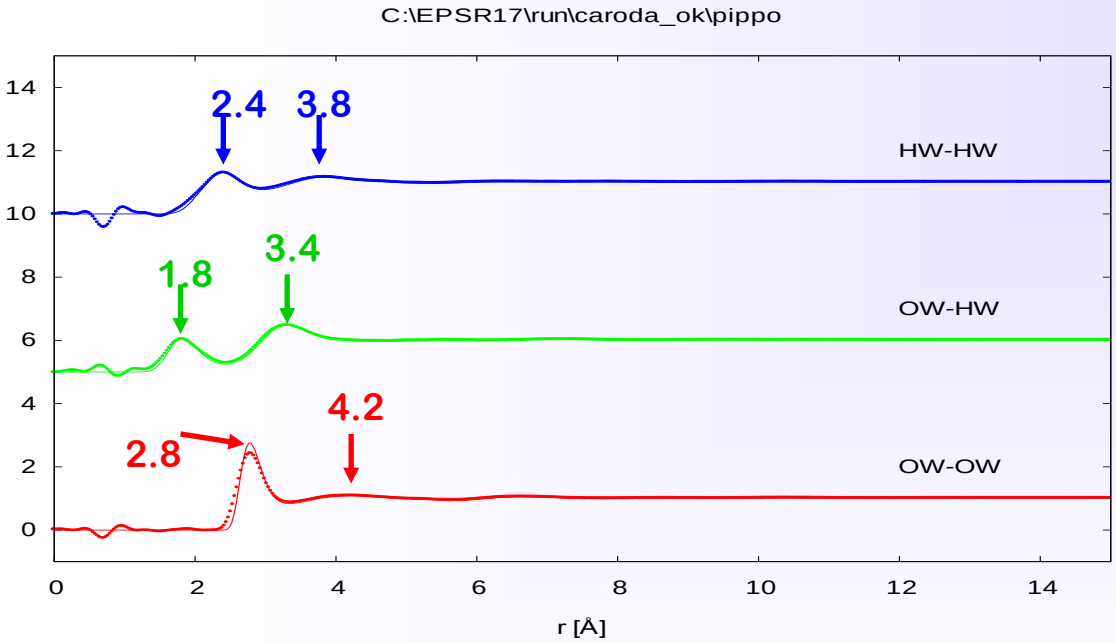

The differences have no structures

## Fit and experimental data



# Analysis Results

## Partial Pair distribution function :g(r)

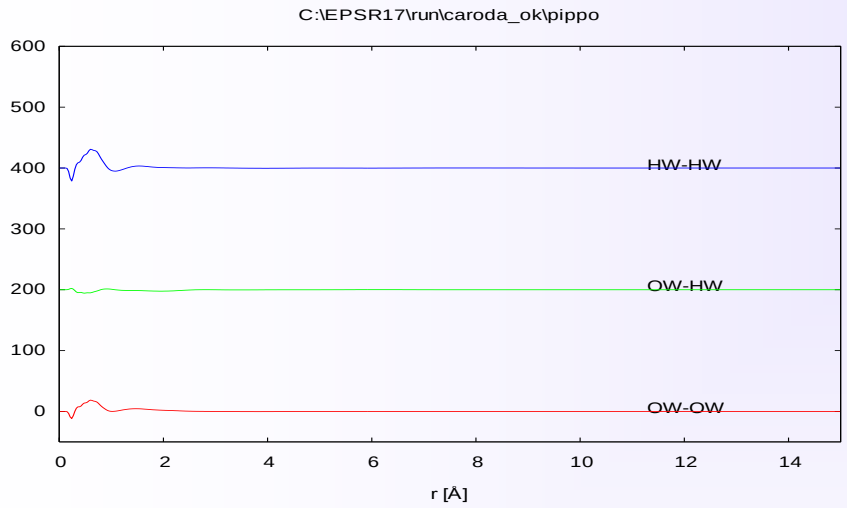



T= 45 °C

- The peaks are at the same position then the water at ambient T
- There are no visible difference on the structure respect to ambient T

# Analysis Results

## Empirical potential

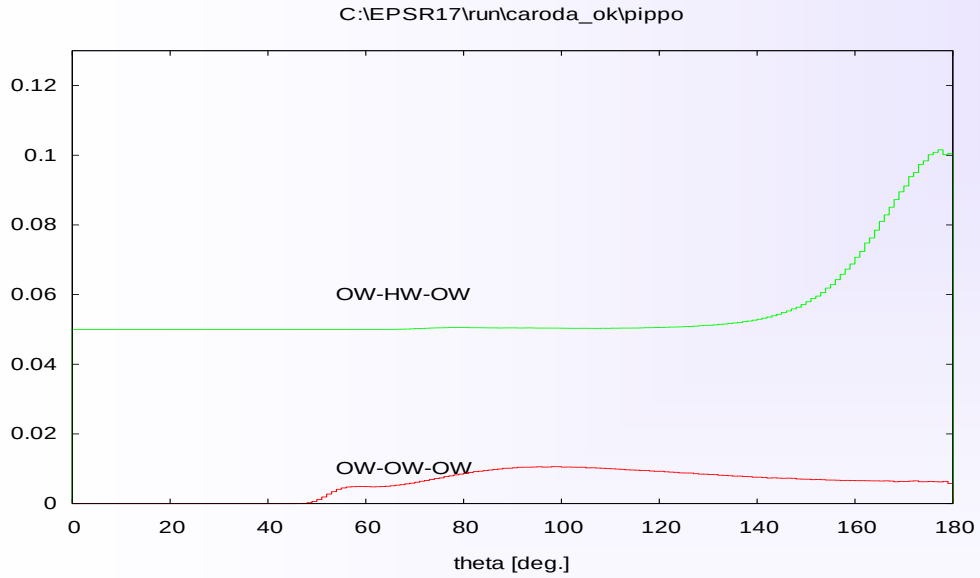


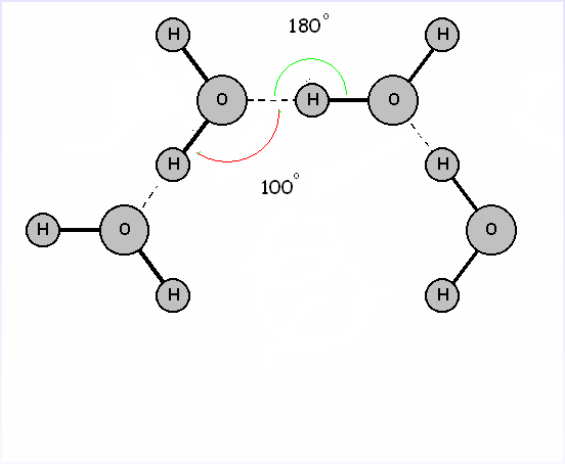

$$U^{ref} = \varepsilon_{\alpha\beta}\left[\left(\frac{r_{\alpha\beta}}{\sigma_{\alpha\beta}}\right)^{6} - \left(\frac{r_{\alpha\beta}}{\sigma_{\alpha\beta}}\right)^{12}\right] + \frac{q_\alpha q_\beta}{4\pi\varepsilon_0 r}$$

- **The correction to the reference potential is very small**

# Analysis Results

## Angle distribution function

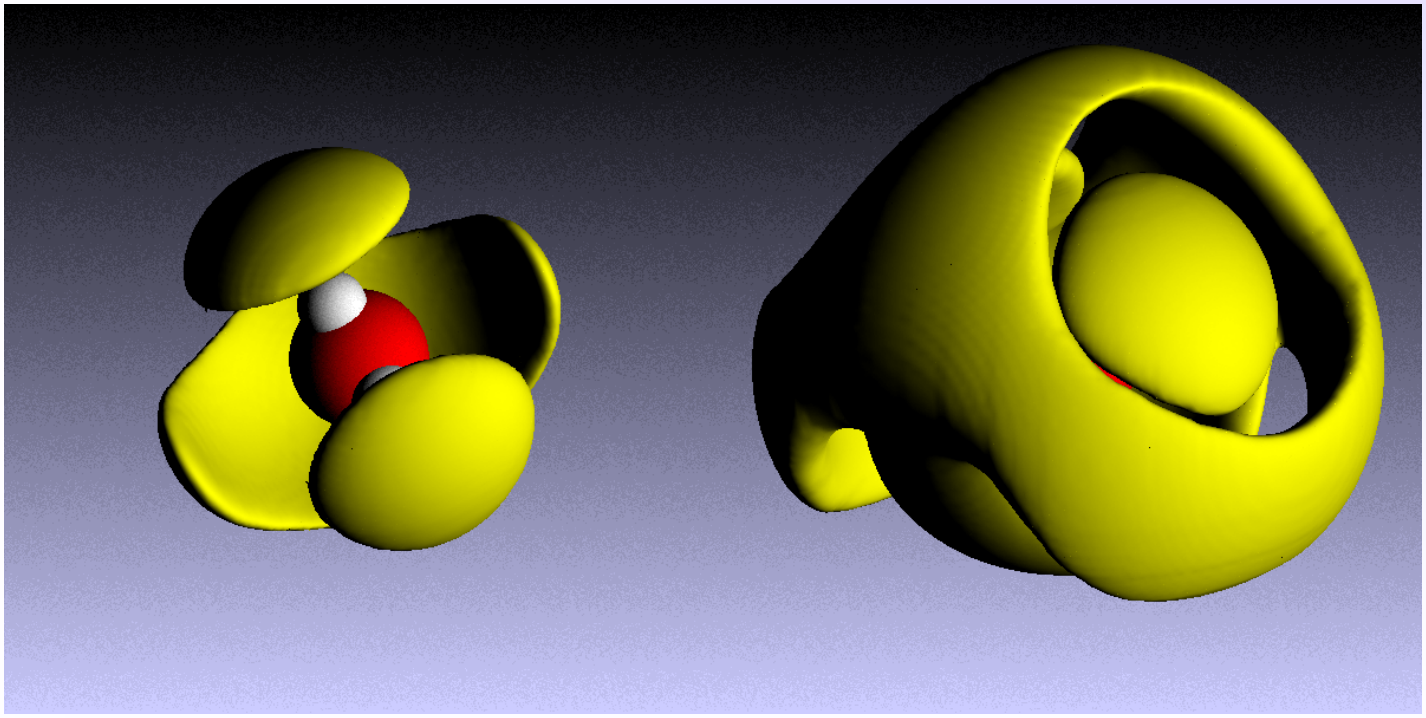



- The O-H-O maximum at $180^0$ represents the H bond
- The O-O-O maximum around $100^0$ describes the tetrahedral structure

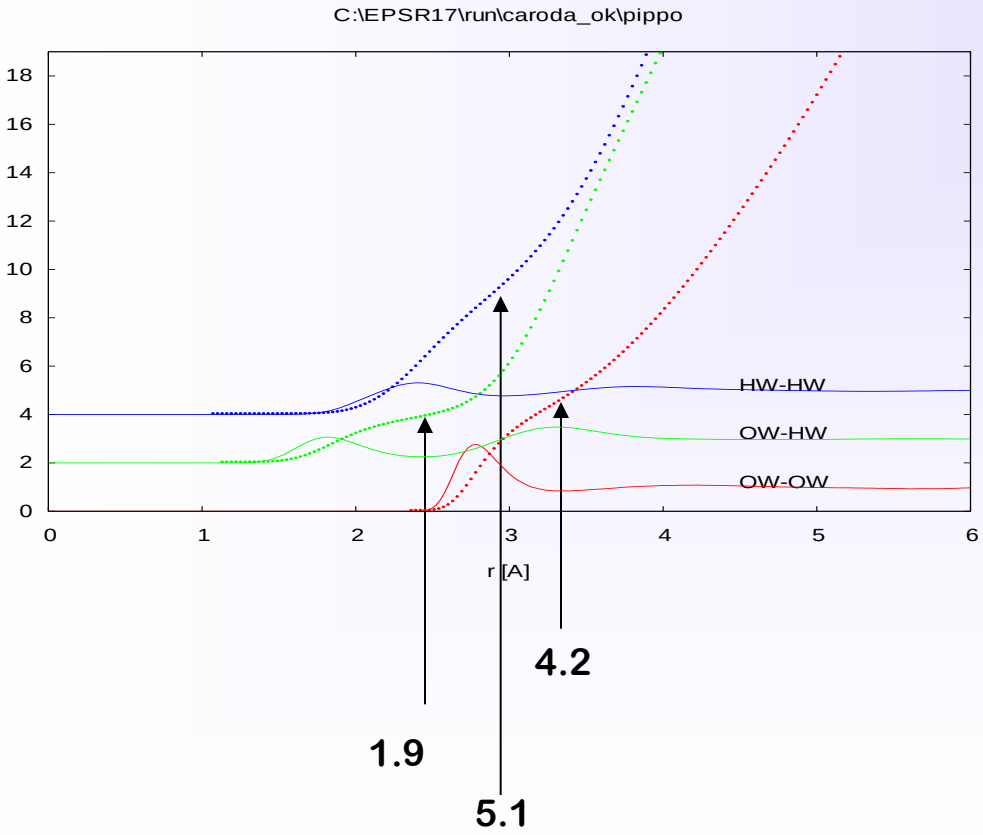
# Analysis Results

**Spatial density function**



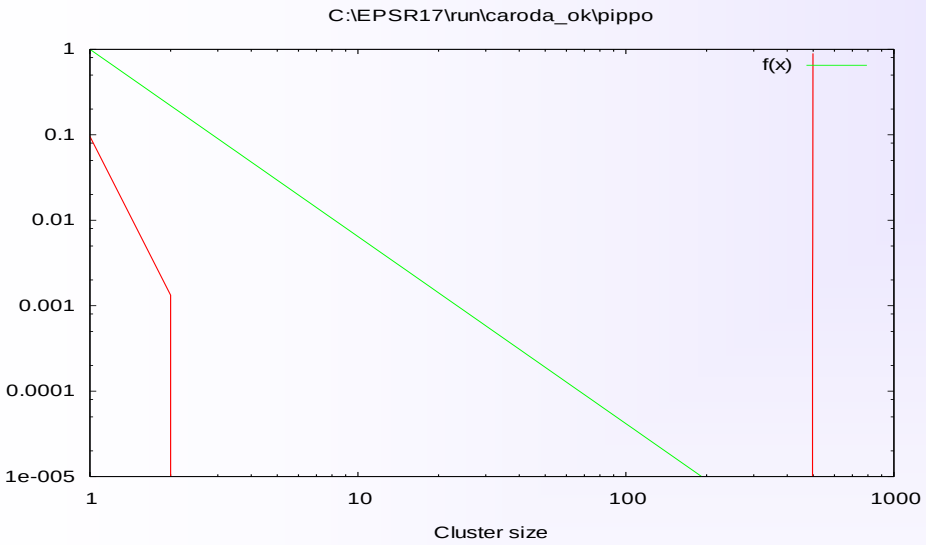
# Analysis Results

## Coordination Number



# Analysis Results

## Water Percolation function




N = 3.9

- There is the evidence of the formation of a big cluster of almost all molecules of the box. We can say that the water is percolating

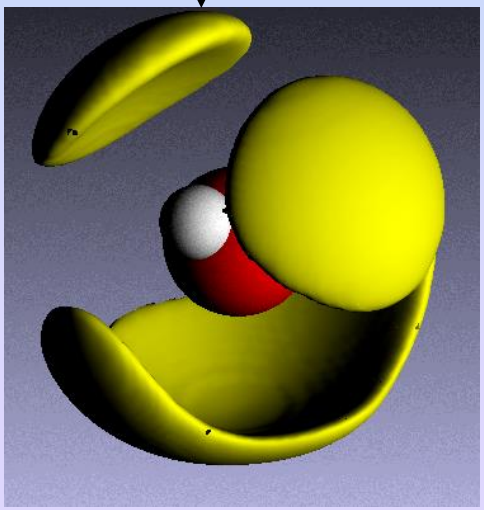
# Conclusions

**We carried out a data analysis on a sample of water at 45 $^0$C using Gudrun and EPSR**

- **At this T the water still present an ordered tetrahedral structure**
- **There is the evidence of the presence of a lot of H bonds**
- **Fitting our data with a box of 500 molecules we can see a big cluster of almost all the molecules ⟹ Percolation**
- **The water structure do not show evident differences with ambient T water**

# Acknowledgements


- Our teachers Silvia Imberti and Rosaria Mancinelli
- The IX school of neutron Scattering "Francesco Paolo Ricci"
- All the speakers
- The band of Baretto


The end
Thank you for your attention!