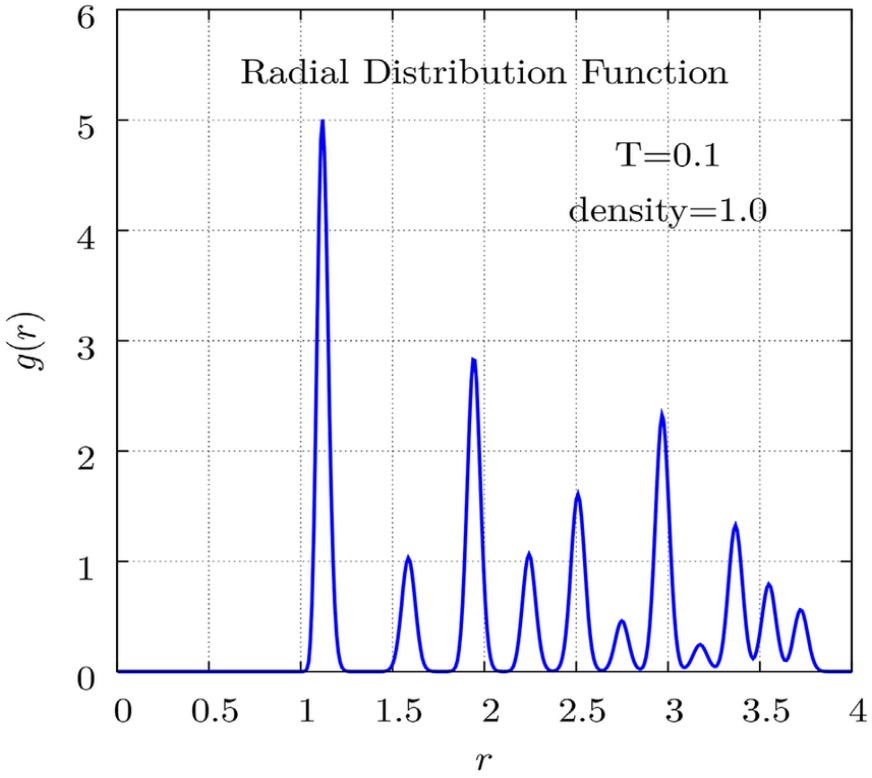
Lab session 5: Liquids

MSE421-Statistical Mechanics

Radial pair distribution function $g(r)$

Why is it important?

- Microscopically (statmech) defined function that can be measured experimentally
- Spatial distribution of atoms
- Connected to other macroscopic quantities (reversible work theorem, energy theorem, virial coefficient)



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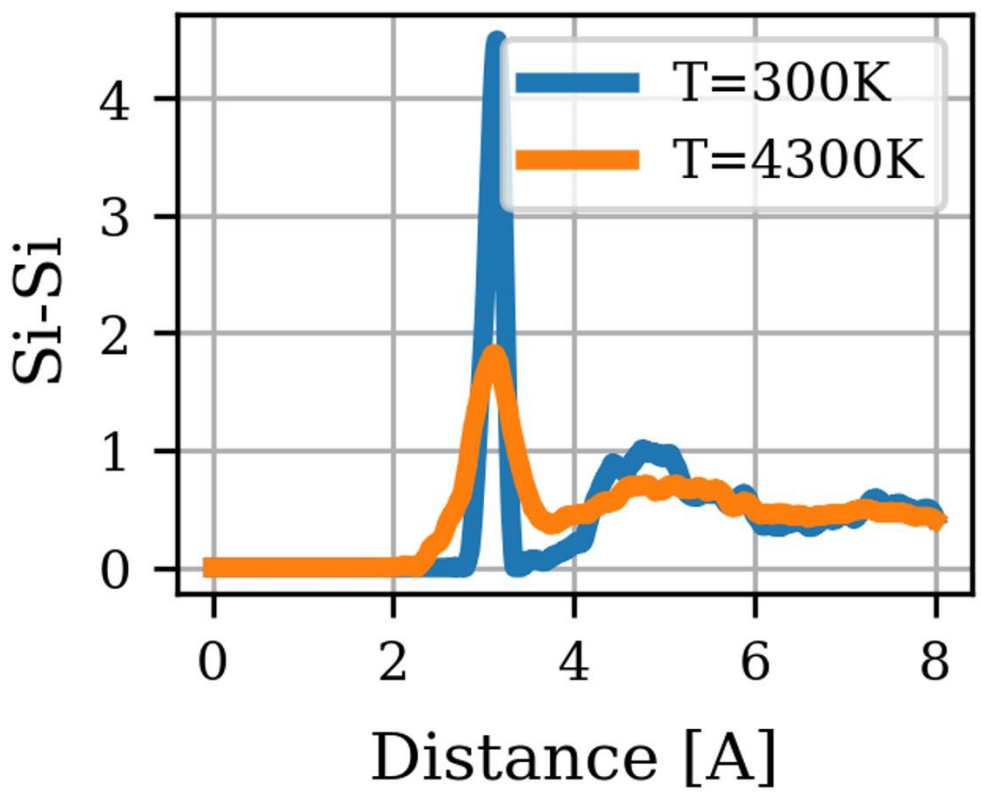


Goal of this exercise session

- Understand $g(r)$
- Gain a better understanding of the phases of matter, with special focus on the liquid phase

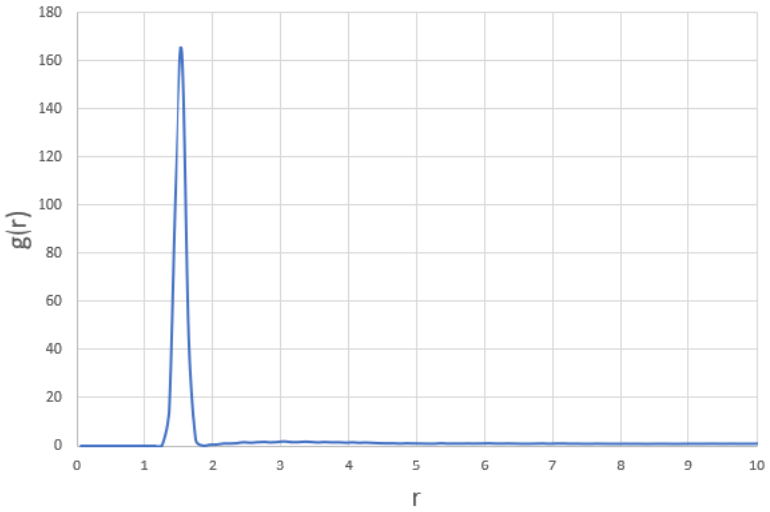
Provided files

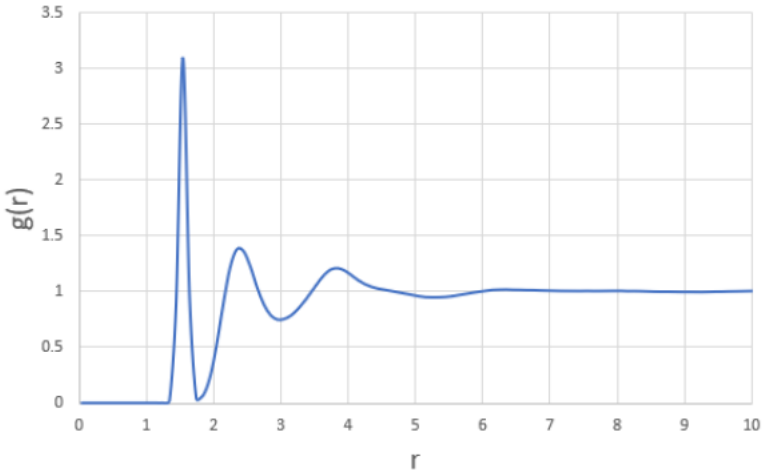
Four different trajectory files of H_2O corresponding to

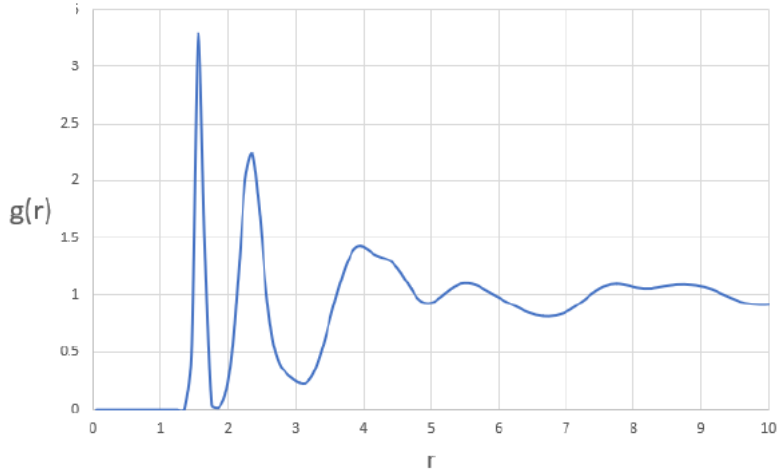
- Solid at 273K
- Liquid at 300K
- Liquid at 580K (high pressure)
- Gas at 580K

Goal: Compare the three phases solid/liquid/gas and how the pair distribution function depends on the temperature

Three Hydrogen-Hydrogen pair distribution functions $g_{HH}(r)$







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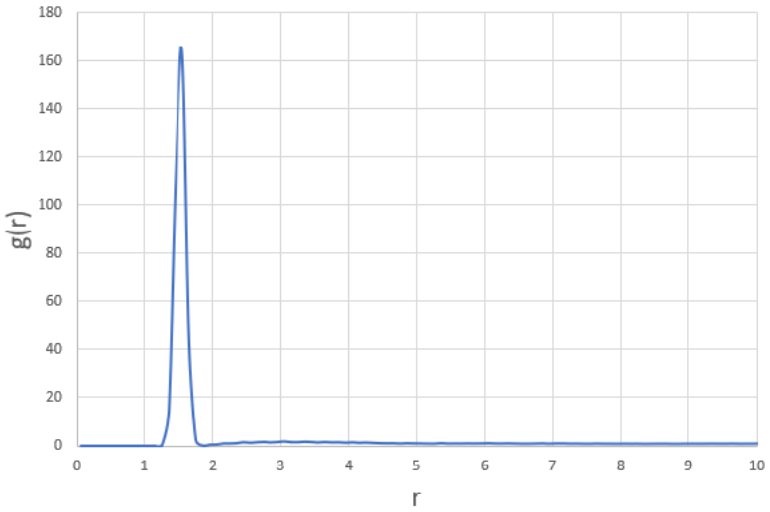
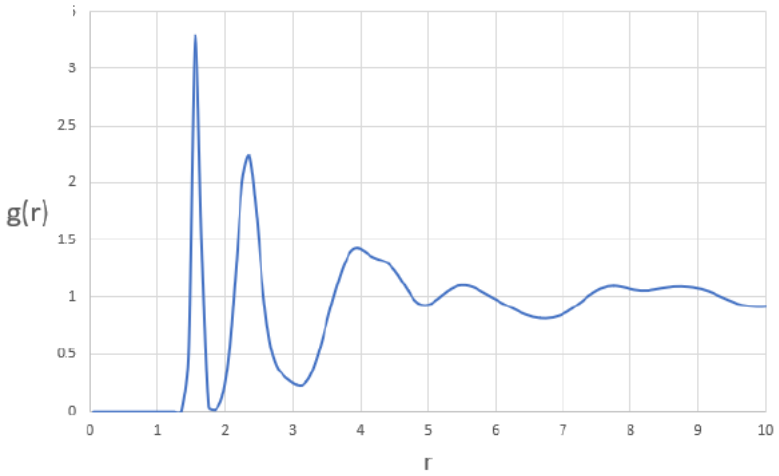
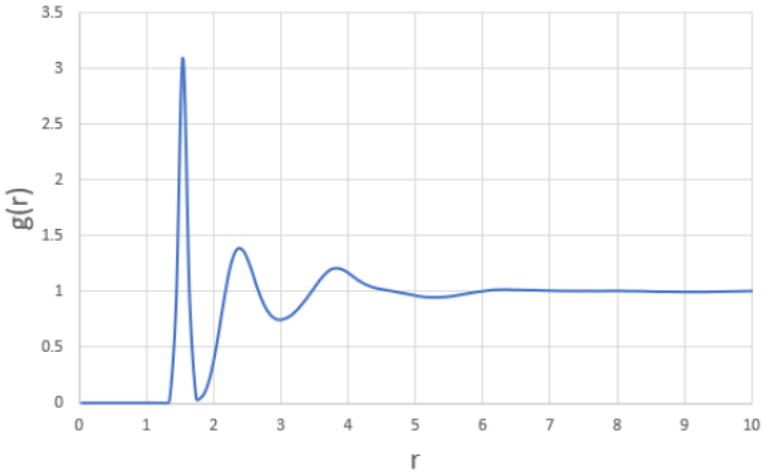


Gas

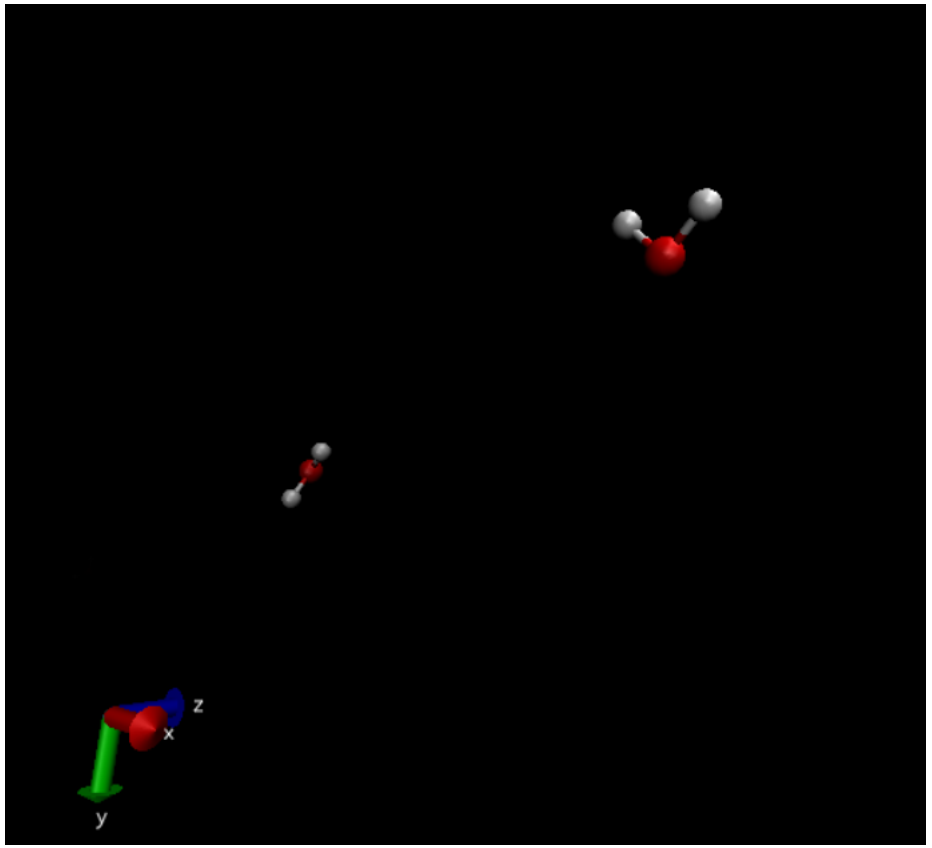
Solid



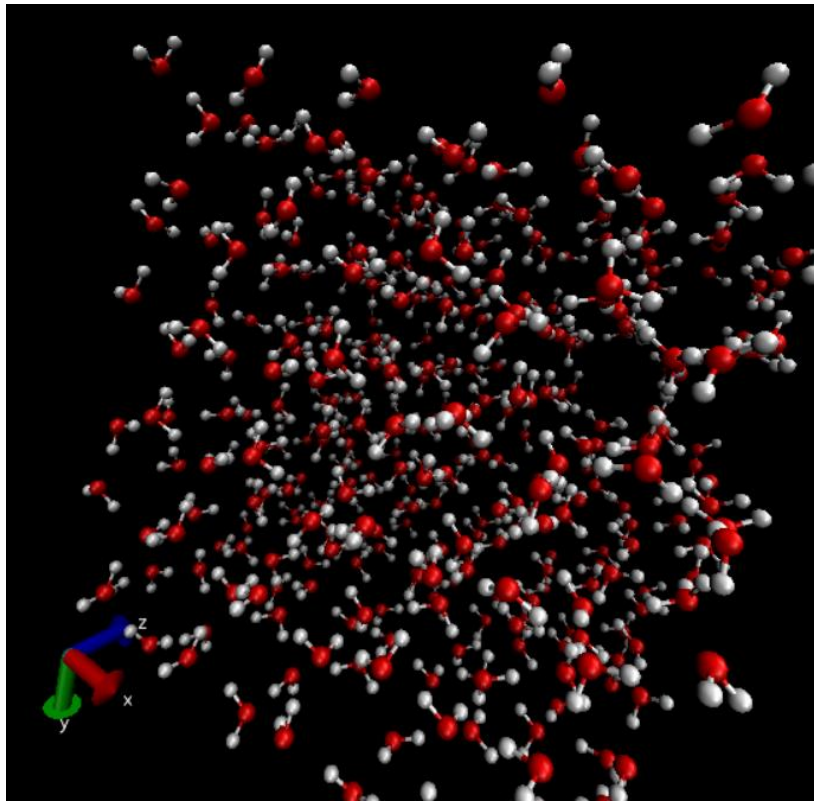


Liquid (close to freezing point)

Gas vs Solid



Gas



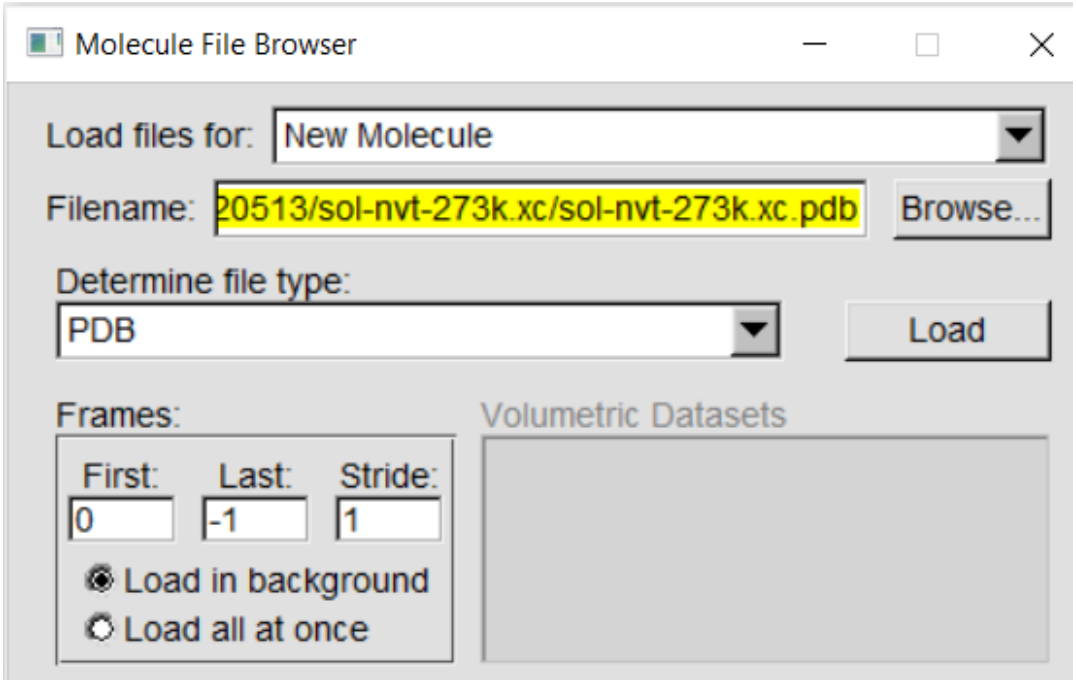
Solid

How to load files

In the main window, choose:

- File → New Molecule

A new window will pop up. Click on browse and choose the desired trajectory file (e.g. “sol-nvt-273k.xc.pdb”)

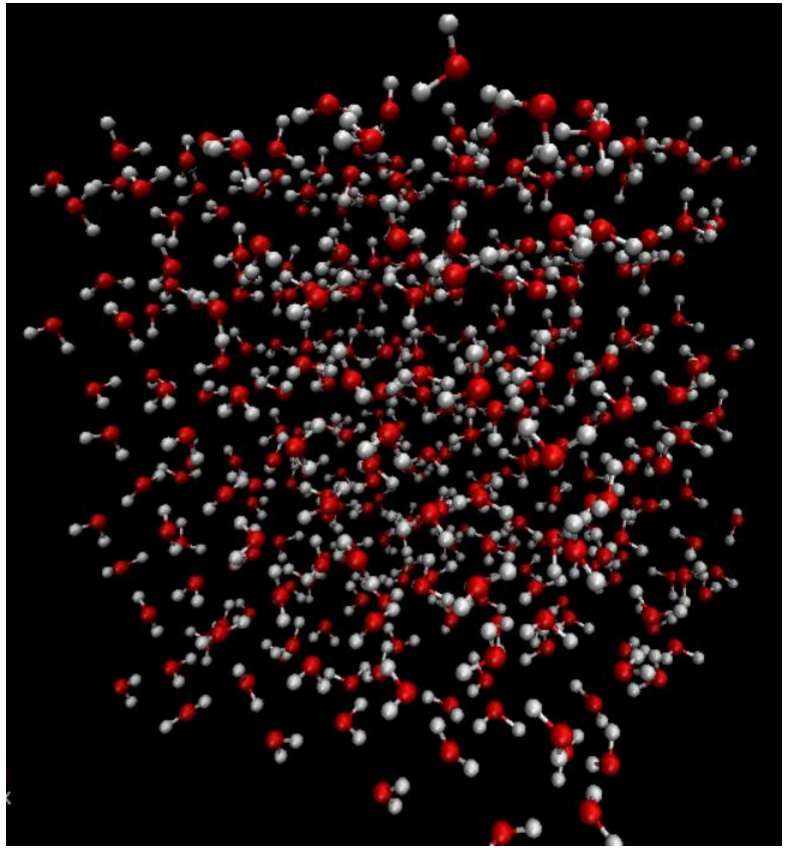


How to change the visual representation

In the main window, choose:

- Graphics → Representations

A window will pop up. In the “Drawing methods” tab, select the desired option, e.g. “CPK”.



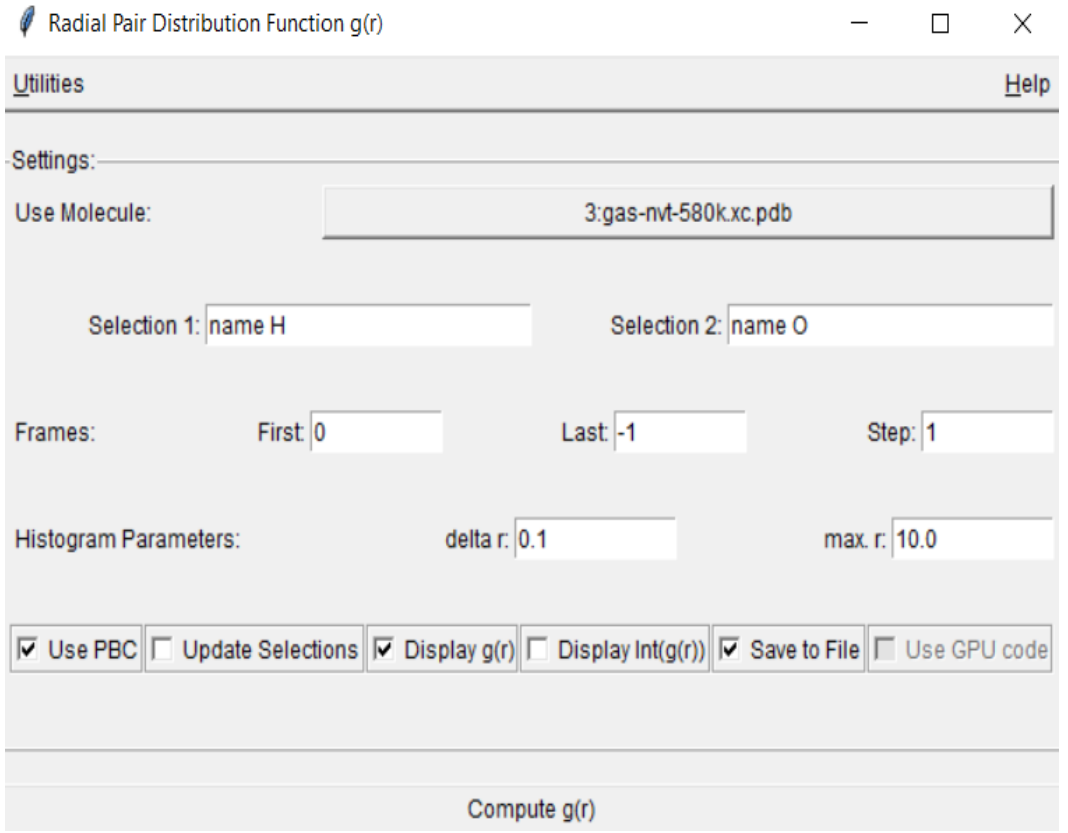
How to obtain the radial distribution function

In the main window, choose:

- Extensions → Analysis → Radial Pair Distribution Functions g(r)

A new window will pop up. To get the Oxygen-Hydrogen pair distribution $g_{OH}(r)$ for the solid phase:

- Select the file “sol-nvt-273k.xc.pdb”
- Type “name O” and “name H” in the boxes “Selection 1” and “Selection 2”.
- Click “Compute g(r)”.



How to compute distances between atoms

In the main window, choose:

- Mouse → Label → Bonds

Now, clicking with the mouse on two atoms will display the distance between them.