Computational Chemistry 2, CHEM-E4225, Exercise 3 9.11.2023

To run Orca you need to load it: module load orca

to run it (in mylly2.pub.chemistrylab.aalto.fi) jsub orca H2O.inp

for cp2k: jsub -np 12 cp2k md-w31-cl.inp

There are a lot of example file in /home/kari/CC2-2023-examples

To see what is in this dir type ls -l /home/kari/CC2-2023-examples (ls is the list command)

you can copy the example files to your own directory: cp /home/kari/CC2-2023-examples/xxx.inp . (there is a dot at the end it is your working directory)

1) Do a calculation of water dimer with PBE. Use ma-def2-TZVP basis. You may want to use the van der Waals correction (D3BJ). What is the binding energy. (for this you need the water monomer energy). Do the frequency calculations for water molecule and dimer. Compare the energy and Free energy. What is the temperature in these calculations?

2) Do a solvation calculation of a water, Na+ and Mg2+ ions. Do the calculations using water and THF as solvent. Does the dipole moments of the water molecule change? Use the CPCM-SMD models. What is the solvation energy in these cases. The CPCM energy is in one line and CDS in another. (There is also Free-energy (cav-disp). This is the cavity term from the CPCM – confusing, see manual chapter 9.27, just use the CDS). Compare the energies of these different systems. What can you say of the dependence of charge and size of the molecules?

3) Do a vibrational calculation for a water and methanol molecules using water as solvent. Do the frequencies change?

4) Do a short (0.5 ps) AIMD simulation of Cl- (or Na+) in water using the CP2K code. How the waters are oriented around the Cl- (or Na+). Here the simulation time is so short that it may be difficult to see the orientation in detail. These simulations will take some hours. (The input file for CP2K is md-w31-cl.inp use 12 cores. The CP2K have to be loaded with command module load cp2k, use ase gui to visualize the w31-cl-pos-1.xyz file) Look the w31-cl-1.ener file for the temperature. You can plot the temp with gnuplot: first gnuplot then inside gnuplot plot 'w31-cl-1.ener' u 2:4 w l (you may need
   You need two files: md-w31-cl.inp and w31-cl.xyz (or similar with na)
   There are also longer Cl simulation files on examples dir if you like to analyse them.

ase-gui can be started with 'module load python'

The instructions of mylly2 are included.

In the first time make your own directory in /home/kari/CC2-2023-results
mkdir /home/kari/CC2-2023-results/ossi (ossi should be your own name)
At end of exercise copy the results to your result dir: cp *out /home/kari/CC2-2023-results/ossi

Orca input library: https://sites.google.com/site/orcainputlibrary/home