Computational Chemistry 2, CHEM-E4225, Exercise 4 7.10.2021

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

to run it (in Wihuri) jsub -np 4 orca H2O.inp

There are a lot of example file in /home/kari/CC2-2021-example

To see what is in this dir type ls -l /home/kari/CC2-2021-example (ls is the list command)

you can copy the example files to your own directory: cp /home/kari/CC2-2021-example/h2o.inp .
(there is a dot at the end it is your working directory)

1) Do NMR calculations of propionic acid, ethanol and TMS (tetramethylsilane) with PBE model and TZVPP basis. Compare the results to lecture notes. Use also B86 DFT model. Note that there are a lot number in the NRM output. The relevant numbers are the Isotopic values at the end of the output file.

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 molecules 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 ethanol molecules using water as solvent. Does 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 ca be loaded with command module load cp2k, use ase gui or vmd to visualize the w31-cl-pos-1.xyz file) Look the w31-cl-1.ener file for the temperature.

ase-gui can be started with 'module load python/3.8-gpaw'

The instructions of Wihuri are included.

In the first time make your own directory in /home/kari/CC2-2021-results
mkdir /home/kari/CC2-2021-results/ossi (ossi should be your own name)
At end of exercise copy the results to your result dir: cp *out /home/kari/CC2-2021-results/ossi

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