

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 a solvation calculation of a water, ethanol molecules and 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?
- 2) Do a vibrational calculation for a water and ethanol molecules. Using water as solvent. Does the frequencies change.
- 3) What is the complexation energy of Na⁺ and water in gas phase and in Na⁺ solvation energy in water. Which of them is larger and why? Compute the energies of water, Na⁺ and Na⁺(H₂O)₆ in gas.
- 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 can 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 ase'`

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>