Setting up the software and running a trial calculation

Read the document on software installation, https://hj.hi.is/reikniefnfr/SettingUpTheSoftware.pdf.

- Install the 150 day free trial version of ChemCraft from the web page https://www.chemcraftprog.com/
- Connect to the Elja computer cluster, at elja.hi.is. Students using laptops with Windows operating system need to set up the program MobaXterm (to get a terminal window) and Xming (to get X11 graphics). Students using laptops with Linux or MacOS operating systems can simply open a terminal window. To log on Elja, type 'ssh -X username@elja.hi.is'.
- Change your login password on Elja with the command 'passwd'.
- Create a folder in your home directory and name it CompChem (Remember: do not use spaces or Icelandic letters in names of directories). Go into the directory by typing 'cd CompChem'.
- Create a sub-directory (inside CompChem) and name it 'lab1'. Go into the sub-directory.
- Copy a jobscript for ORCA from the TA's directory, 'cp /users/home/share/CompChem/lab1/sub.sh .' and check to make sure the file has been copied to your directory by using the ls command.
- Copy an input file for the ORCA program, 'cp /users/home/share/CompChem/lab1/orca.inp .' into the same directory.
- Open the file 'orca.inp' with text-editor nano by typing 'nano orca.inp' and inspect the file. It is an energy and gradient evaluation ('ENGRAD') of a water molecule using Hartree-Fock theory. Then exit the file.
- Submit this calculation to Elja by typing 'sbatch sub.sh'.
- Wait for the calculation (or job) to finish. You can monitor it by typing 'squeue -u username'.
- Inspect the ORCA output file. Find the 'final single point energy' of the water molecule.
- Download the ORCA output file to your local machine and open it with ChemCraft.
- Inspect the geometry of the molecule. Play around with ChemCraft. Try rotating and moving the molecule, use different styles to depict the H_2O geometry, label the atoms, measure Cartesian distance between the atoms and angle etc.
- What is the angle of the water molecule?