Computational Chemistry 1, CHEM-E4110, Quantum chemistry I 9.1.2018

Here are some instruction how to use some tools needed in the Computational Chemistry course

Putty and Xmin.

The easiest way to connect to wihuri is to use putty and Xming. The address of wihuri is **wihuri.pub.chemistrylab.aalto.fi**. You need first to start Xming (from program list of a Windows machine). Click the Xming icon. Then start Putty. The connection need to be SSH. You need also to start the X11 connection. That can be found in the SSH line (click the + sign). Then click the X11 line and from it select the Enable X11 forwarding.

Then go back to the Session and copy the wihuri address to the address line. After that you should get a black-background window to wihuri. Put you username and password to it.

ChemDraw and Chem3D

ChemDraw is an easy to use program to draw 2D molecules (or molecular sketches). It has tools to do most of the molecules chemist are interested. For us the Chem3D is more useful. It have also the drawing facilities and it will also handle the 3D structures. Try it. For Orca we need to have the .xyz file. So far I have not found a correct xyz file format. You can save the coordinates as Tinker MM2, or cart coord format. To copy the file I have used WinSCP and open a connection to wihuri. I just drag the icons to wihuri. There might be more convenient ways.

Editors

You need to edit several file and for that you need some editor. It is better to use some unix editors since Word will (can add some special characters to the file). There a several editors like gedit, emacs, nano, etc.

xyz file format: first line – number of atoms, second line – comments or empty, third as so on – atom label (like C, O, H, Na) and x, y and z coordinates.

Unfortunately the Chem3D do not produce correct xyz file. One need to edit the Cartesian coordinates file.

Orca

One need first to load orca: module load orca

Make some input file. Like h2o.inp. there are several examples in /home/kari/CC-examples

There is also an excellent and large input library for Orca. It complements well the manual.

https://sites.google.com/site/orcainputlibrary/home

Run Orca with 4 cores. (for small molecule you can leave the –np out and do not use more than 12 cores.)

jsub –np 4 orca name.inp

The output will become to name.oout. Learn to read the oout files. Look also name.trj file

see what is going on jstat

gpaw

One need first to load gpaw: module load gpaw

module load gpaw-utils

module load ase

Make some input file. Like cu.py. There are several examples in /home/kari/CC2-examples

Run gpaw with 4 cores. (for small molecule you can leave the –np out and do not use more than 12 cores.)

jsub –np 4 gpaw name.py

The output will become to some name you have specified in the .py file.

see what is going on jstat

ag (ase-gui)

A simple graphical visualization tool. it can be loaded with command: module load ase

then one can visualize .xyz files as

ag h2o.xyz or h2o.trj.xyz (do first cp h2o.trj h2o.trj.xyz , .trj file contain xyz coordinates during the optimization)

the ag can also be used for simple molecular manipulations.

Simple Linux commands

mkdir - make a directory example: mkdir kariLaa, or mkdir harj-1

cd – change directory example cd kariLaa

ls , ls –l - list files (also ll do the same thing) example ls /home/kari/CC-examples also ls ../

cp file1 file2 - copy file1 to file2, example cp h2o.inp h2o.inp.save

more file - type a file to screen example more h2o.oout

tail file or tail -100 file - last 10 or 100 lines of a file example tail h2o.oout

grep XXX h2o.oout - find and print lines that contain XXX (Note Linux is case sensitive)

example: grep FINAL h2o.oout

Some www pages of Linux commands:

http://www.dummies.com/computers/operating-systems/linux/common-linux-commands/

http://www.comptechdoc.org/os/linux/usersguide/linux_ugbasics.html