Computational Chemistry II, CHEM-E4110,   Quantum chemistry II   2022

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

Putty and Xming/Xload.

The easiest way to connect to mylly2 is to use putty and Xming. The address of mylly2 is **mylly2.pub.chemistrylab.aalto.fi**.

NOTE: there was problems to login to mylly2 from the Kandi-centre computer class. One can login first to kosh.aalto.fi. Remember to set the X11 also before that. The passwd tp kosh is you Aalto passwd. From kosh one can login to mylly2 with

ssh student1@mylly2.pub.chemistrylab.aalto.fi -X   (or student2,3 etc)

The -X allows you to use the X-windows. mylly2 will ask its own passwd.

Instructions to mylly2

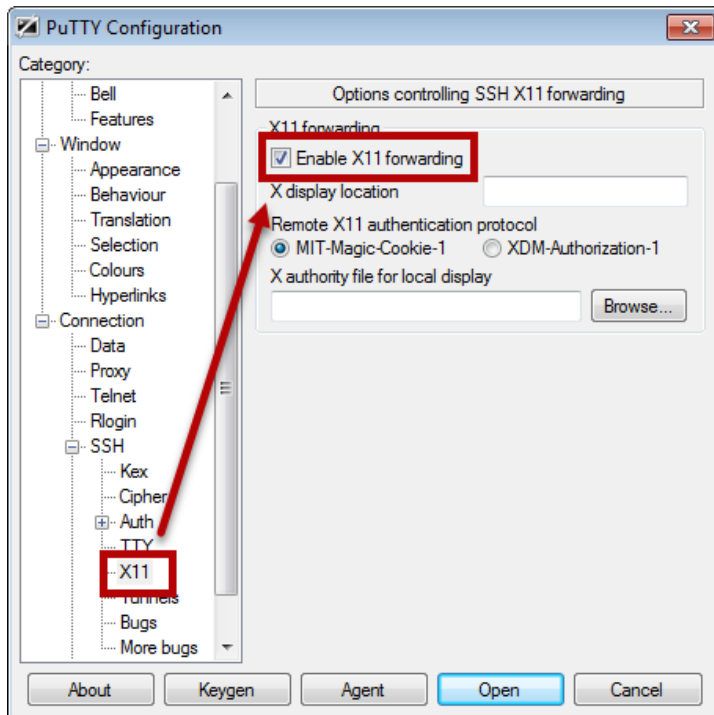https://wiki.aalto.fi/display/IMM/Mylly2+Quick+Start+Guide

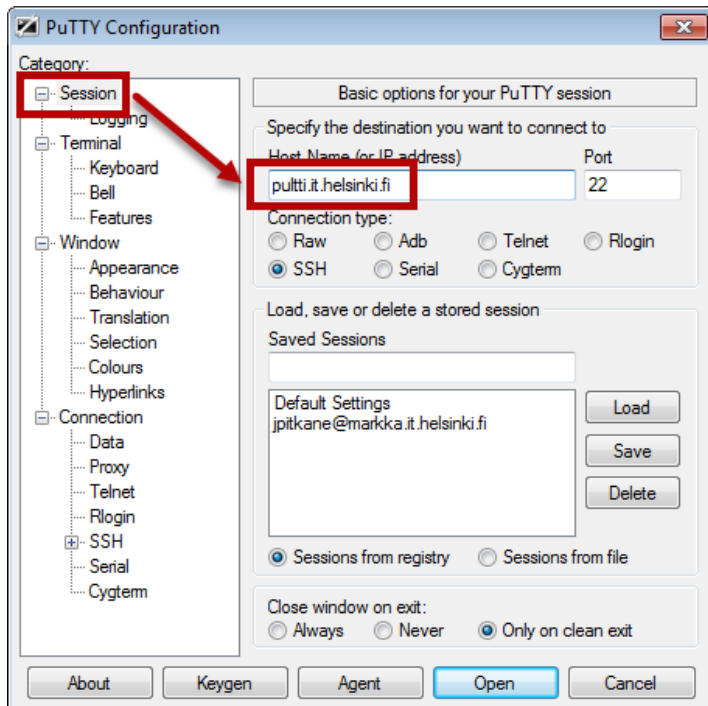You need first to start Xload (from program list of a Windows machine). Click the Xload icon.

see also

https://helpdesk.it.helsinki.fi/ohjeet/tietokone-ja-tulostaminen/ohjelmistot/x-ikkunointi-xming-ohjelman-avulla

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 mylly2 address to the address line. After that you should get a black-background window to mylly2. Put your username and password to it.
You should also save the session so you do not need to give the name every time.

Making structures

ase gui

ase gui in mylly2 is a simple tool to show and manipulate molecules. (for the later it is very clumsy.) The default is not very nice but if you Show bonds (in View menu or Ctrl-B) it is nicer.

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.

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 add some special characters to the file. There are several editors like gedit, emacs, nano, etc.

example: nano Cu.py (or nano h2o.inp)

write the file ^O exit ^X see the bottom line

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.

gpaw

One need first to load gpaw: module load python/3.8-gpaw

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

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 example: jsub –np 4 gpaw Cu.py

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

 see what is going on jstat and ls –l Cu*out (list all the files that start with Cu and to out)

(versio 5.0)

module load orca

Make some input file. Like h2o.inp. There are several examples in **/home/kari/CC2-2022-examples**

jsub –np 4 orca xx.inp   example: jsub –np 4 orca h2o.inp

This will used 4 cores is you need more memory jsub -np 4 -mem 2G orca some.inp

The output (will end at .out) will become to some name you have specified in the .inp file.

see what is going on jstat   and ls –l h2o*

ase (ase gui)

A simple graphical visualization tool. load it   module load python/3.9-2022-10

then one can visualize .xyz files as

ase gui h2o.xyz   or   h2o.trj.xyz

the ase gui can also be used for simple molecular manipulations.

Simple Linux commands

. is the present dir   .. on dir above

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

cd – change directory   example cd kari   or cd /home/kari/CC-new-results

ls , ls –l - list files   (also ll do the same thing) example ls /home/kari/CC2-2022-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.out

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

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

example: grep FINAL h2o.out

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

Machine learning

use first module load python/3.9-2022-10

python some.py

WinSCP

is a graphical program that can be used to copy files from you PC to mylly2. Start it from WinSCP command and login to mylly2. You need to whole name and save it for further uses. After it is open you can drag the files to and from mylly2. Use your desktop for source files.