

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

Putty and Xming/Xload.

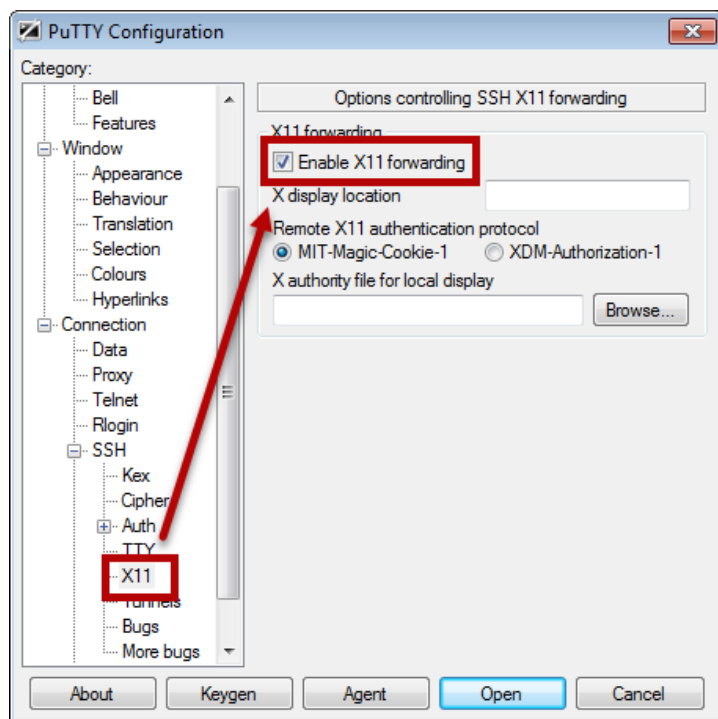
The easiest way to connect to wihuri is to use **putty** and **Xming**. The address of wihuri is **wihuri.pub.chemistrylab.aalto.fi**. You need first to start Xload (from program list of a Windows machine). Click the Xload icon.



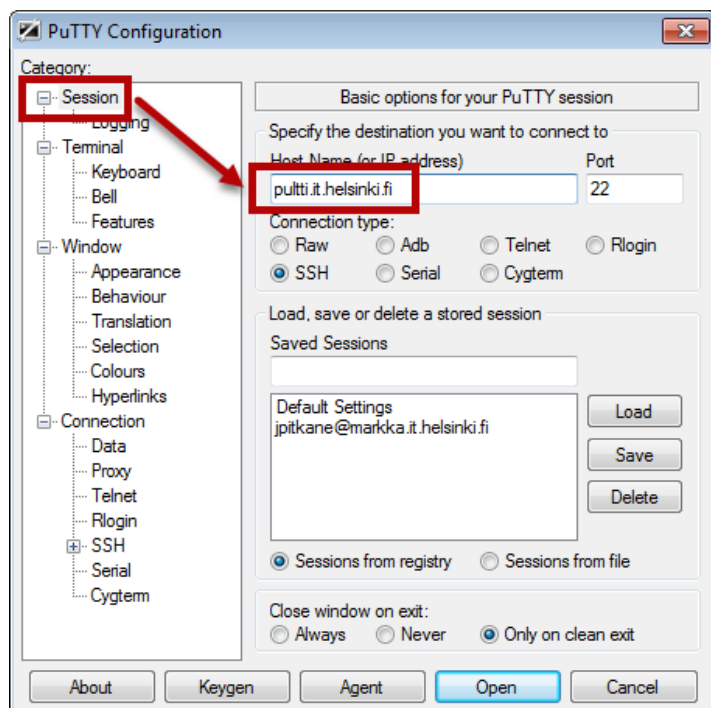
see also

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

Then start Putty. The connection needs 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 your username and password to it.



Making structures

ase

ase gui or ag in wihuri is a simple tool to make bulk and surface structures. Most of the command are in the gpaw python but you should try ase gui and the Setup command

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)

orca

module load orca

Make some input file. Like h2o.inp. There are several examples in /home/kari/CC2-2021-example

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

The output (will end at .oout) 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. it can be loaded with command:

module load python/3.8-gpaw

then one can visualize .xyz files as

ase gui h2o.xyz or h2o.trj.xyz

or VMD (no need to load anything)

vmd h2o.xyz

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

Simple Linux commands

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/CC-new-example 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

