

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

Putty and Xming/Xload.

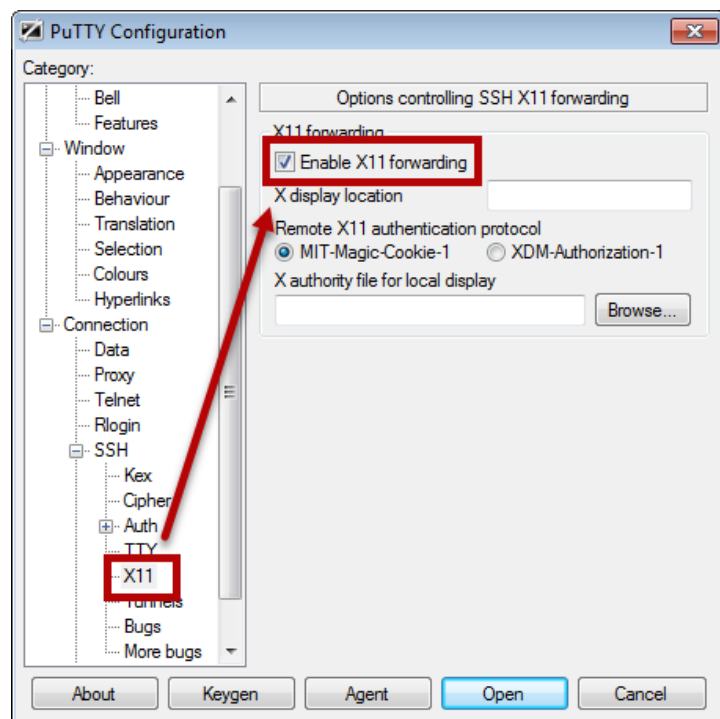
The easiest way to connect to wihuri is to use **putty** and **Xming**. The address of wihuri is **wihuri.pub.chemistrylab.aalto.fi**. You need first to start Xload (from program list of a Windows machine). Click the Xload icon.



see also

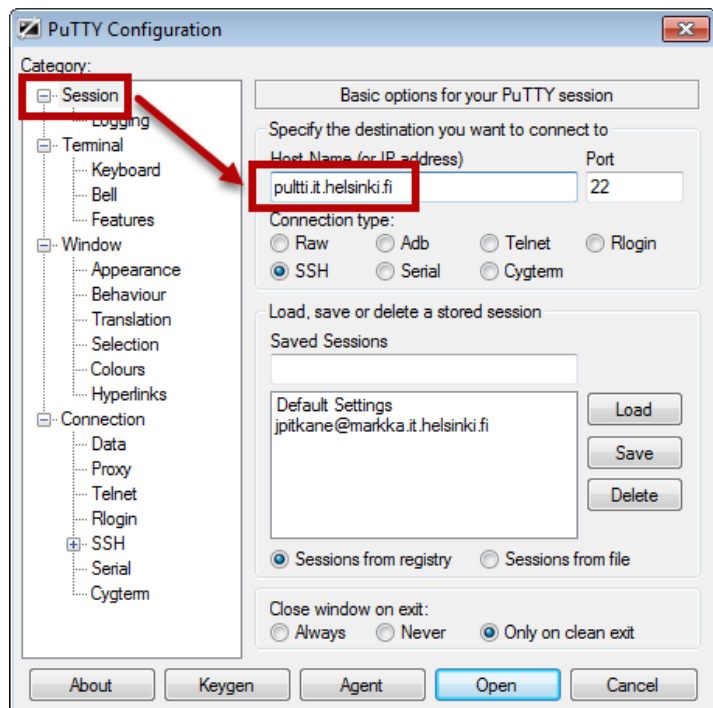
<https://helpdesk.it.helsinki.fi/ohjeet/tietokone-ja-tulostaminen/ohjelmistot/x-ikkunointi-xming-ohjelma-avulla>

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. Save the session so you do not need to type it every time.

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

module load ase

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 files 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

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.

orca

One needs first to load orca: `module load orca`

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

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` example: `jsub -np 4 orca h2o.inp`

The output will become as h2o.oout the same name you have specified in the .inp file.

see what is going on `jstat` and `ls -l h2o*` (list all the files that start with h2o)

ase-gui

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

then one can visualize .xyz files as

`ase-gui h2o.xyz` or `h2o.trj.xyz` (do first `cp h2o.trj h2o.trj.xyz`, .trj file contains xyz coordinates during the optimization)

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