

Software and hardware tools for CHEM545

Fall 2014

Outline

- IQmol: graphic user interface;
- Q-Chem: electronic structure engine;
- HPCC: high-performance computing cluster. All Chem545 students are already added to our HPCC allocation.

IQmol and Q-Chem

- See separate document for step-by-step instructions for how to download, install, and configure IQmol.
- IQmol features contextual help.
- Uptodate Q-Chem manual is available at the chem545 website.
- You should be able to run Q-Chem via IQmol only, without having to log in to HPCC. However, I strongly recommend to learn basic UNIX to be able to login and manually submit jobs at HPCC by using pbs systems. You will also need it to access outputs of long jobs.

Unix basics

- Learn how to make, change directories, move files.
- Learn how to ssh and sftp.
- Learn basic unix editor (vi, emacs, etc) so you can edit text files.

HPCC

- HPCC - High Performance Computing & Communications
- More information <http://www.usc.edu/hpcc/index.php>
- A lot of technical information about the cluster (for advanced users): <http://hogwarts.usc.edu/~krylov/HPCCworkshop.pdf>

HPCC: more details

Our HPCC account (queue) is 'lc_ak'

Each user has a subdirectory matching their user id within our working directory /home/rcf-proj3/ak

Please use head nodes hpc-login1 (32 bit node) and hpc-login2 (64 bit node) for compiling, running small test jobs, and submitting jobs to the queue. Reference HPCC web site for information regarding working on the Linux cluster:

<http://www.usc.edu/hpcc/systems/use-l-o>

For Q-Chem jobs: use hpc-login2 only.

Login to HPCC

- On Windows, you need to download and install SSH client. For example this one: [Bitvise Tunneller](http://dl.bitvise.com/Tunnelier-Inst.exe) (<http://dl.bitvise.com/Tunnelier-Inst.exe>)

After installation open the program and use the following settings:

Host: hpc-login2.usc.edu

Port: 22

Username: your USC account name used for the USC e-mail

Password: your password for the USC account

After you login to HPC you will see two windows:

black one is called terminal and used to type commands

second window is a graphical interface for SFTP that allows you to copy files from you local machine to HPC

On Linux/Mac, simply use terminal and ssh command.

Submitting Q-Chem jobs via pbs

1. Jobs on HPCC should be submitted using PBS queueing system.
2. To submit a job, create a text file 'script.run' (see next slide for the template).
3. Edit script to choose the mode of execution (-nt or -np) and name of the input and output.
4. Submit job by typing: 'qsub script.run'
5. Use qstat to check the status of your job and qdel to delete a submitted job.

script.run file

```
#!/bin/bash
#PBS -q default
#PBS -l walltime=00:30:00
#Edit line below to change the number of CPUs
#PBS -l ncpus=4

source /usr/usc/intel/default/setup.sh
source /usr/usc/openmpi/1.8.1/gnu/setup.sh
export QC=/home/rcf-proj/ak/ikaliman/qchem/trunk
export QCAUX=/home/rcf-proj/ak/ikaliman/qchem/qcaux
export QCPLATFORM=LINUX_Ix86_64
export QCRSH=ssh
export PATH=$QC/bin:$PATH
export QCSCRATCH=$TMPDIR
cd $PBS_O_WORKDIR
#Edit this line to change the name of input and output
#and the mode of execution (should be consistent with ncpus value above)
qchem -nt 4 my_input.inp my_output.out
```

To submit a job, edit this script appropriately and type 'qsub script.run'

Using Q-Chem on HPCC

- Detailed instructions (by Kirill Khistyayev) for experts can be found at:

<http://hogwarts.usc.edu/~kirhist/hpcc/>