IQmol: Server Setup & Job Submission

Shirin Faraji, Ilya Kaliman, and Anna Krylov
Written by Dr. Andrew Gilbert

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Server setup
### Server setup

#### Server List

<table>
<thead>
<tr>
<th>Name</th>
<th>Address</th>
<th>User</th>
<th>Authentication</th>
<th>Type</th>
</tr>
</thead>
</table>

[Image of a server setup window with options for adding a new server.]
This is a setup for USC HPCC cluster, but with small modifications it can be used for other clusters running pbs (such as fluffy).

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

**Password** (will be asked when you test connection): your password for the USC account.
Server setup

Copy from next slide!
#!/bin/bash
#PBS -q ${QUEUE}
#PBS -l walltime=${WALLTIME}
#PBS -l ncpus=${NCPUS}

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
qchem -nt ${NCPUS} ${JOB_NAME}.inp ${JOB_NAME}.out
Submitting job
- Use default queue on HPCC;
- Leave the rest of settings unchanged.

**For advanced users:**
- To run Q-Chem in parallel (openmp), change the number in CPUs *(consult the manual* to see which types of jobs are openmp-parallelized);
- for MPI-parallel, you will need to tweak the settings in the previous page;
- Memory and scratch settings are not important here, but for optimal performance you may need to tweak these settings in the *Q-Chem input file*, especially for advanced calculations. **Consult the manual** before doing so!
Check job status
Job status will be displayed in a new window:

- Use the left mouse button to select the job.
- Use the right mouse button to see this menu.
- Kill the job by selecting this option.
Job is finished
Copy files to your laptop

Note:
Must be the same name as the folder you have created while submitting the job
After you copied files to your laptop

Golden star shows that it is copied properly

Click the checkbox!