

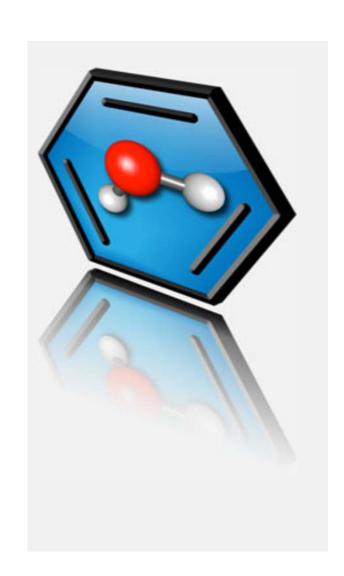
IQmol: Server Setup & Job Submission

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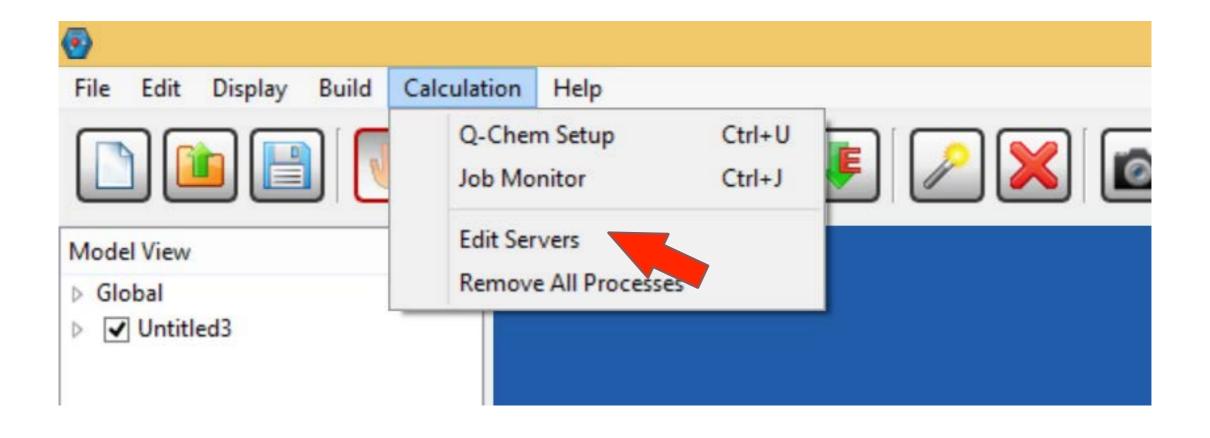


Resources

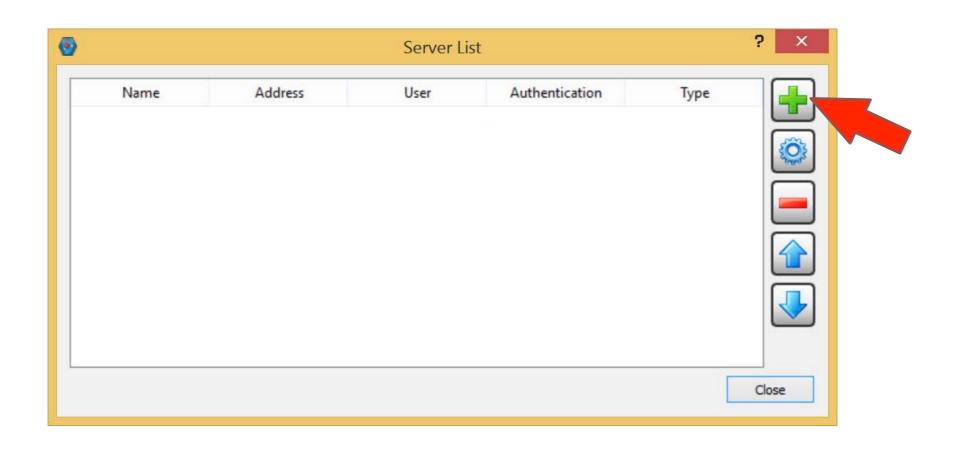
- Written by Dr. Andrew Gilbert
- Keep yourself up to date with IQmol website: http://iqmol.org
- IQmol Youtube channel: IQmol now has its own Youtube channel



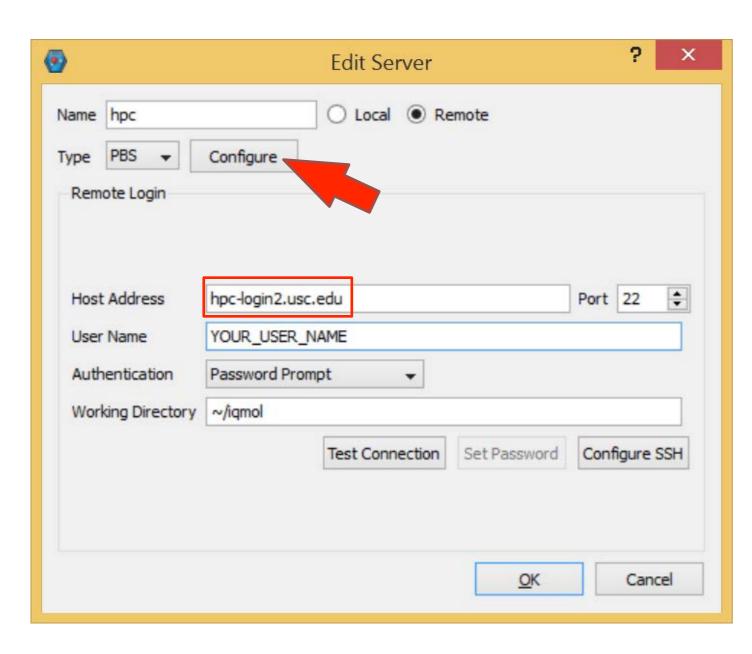












This is a setup for USC HPCC cluster, but with small modifications it can be used for other clusters running pbs (such as fluffy).

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.



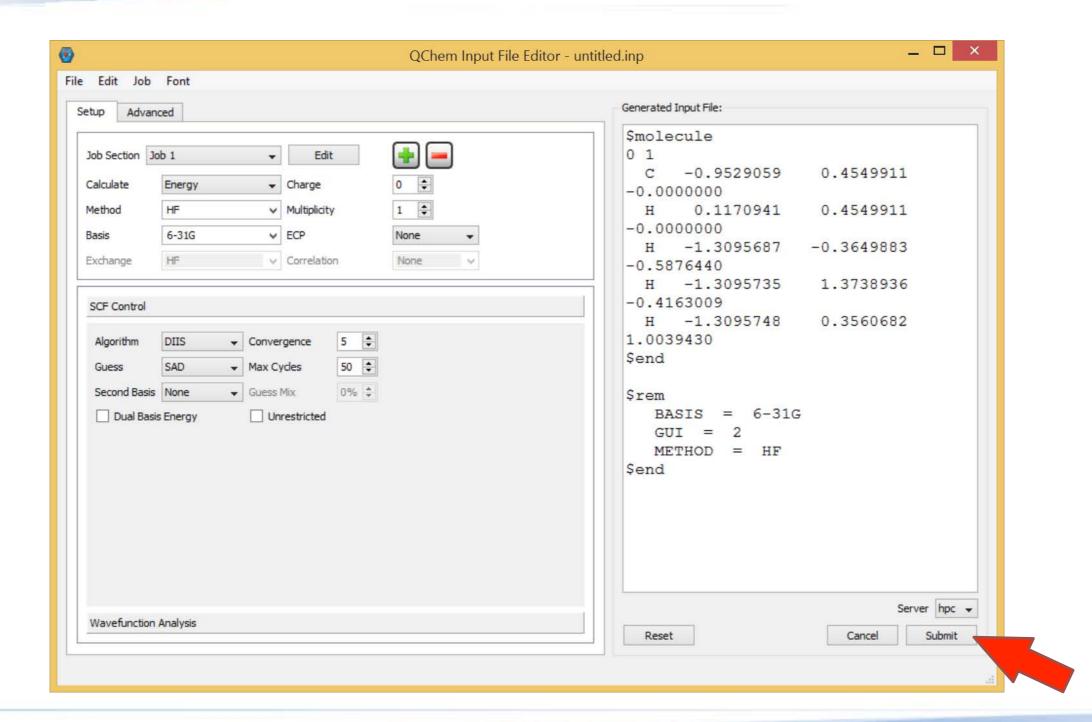
	Server Options		? ×	
Command Settings	s			
\${EXE_NAME}	qcprog.exe			
\${SUBMIT_CMD}	qsub \${JOB_NAME}.run			
\${QUERY_CMD}				
\${QUEUE_INFO}				
\${KILL_CMD}	qdel \${JOB_ID}			
Run File Template				
export QC=/hom export QCAUX=/ export QCAUX=/ export QCRSH=s export PATH=\$Q export QCSCRATI	\${WALLTIME} {NCPUS} ntel/default/setup.sh penmpi/1.8.1/gnu/setup.sh e/rcf-proj/ak/ikaliman/qchem/trunk home/rcf-proj/ak/ikaliman/qchem/qcaux DRM=LINUX_Ix86_64 sh C/bin:\$PATH CH=\$TMPDIR		Copy from next slide!	
pdate Interval 20	s 🛊		OK Cancel	
			OK Caricel	



```
#!/bin/bash
#PBS -q ${QUEUE}
#PBS -1 walltime=${WALLTIME}
#PBS -1 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
```

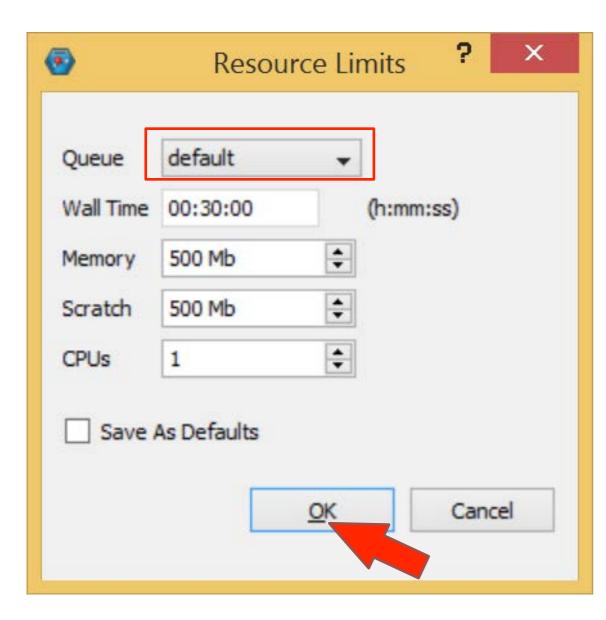


Submitting job





Submitting job



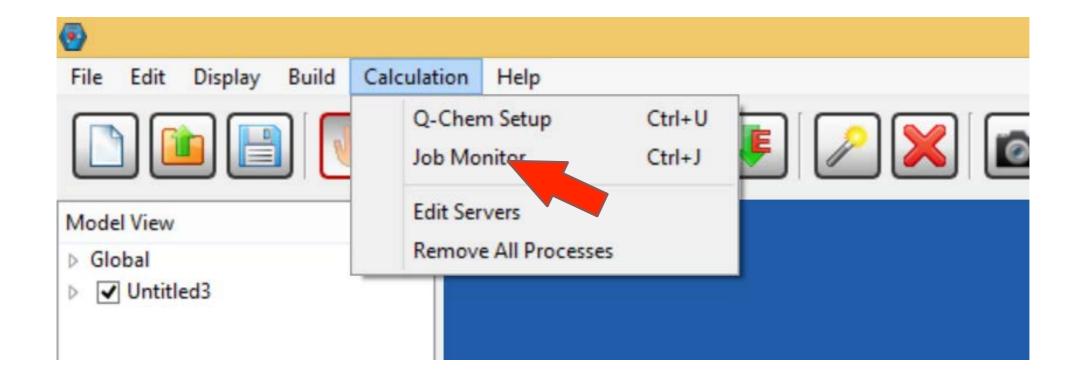
- Use default queue on HPCC;
- Leave the rest of settings unchanged.

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!



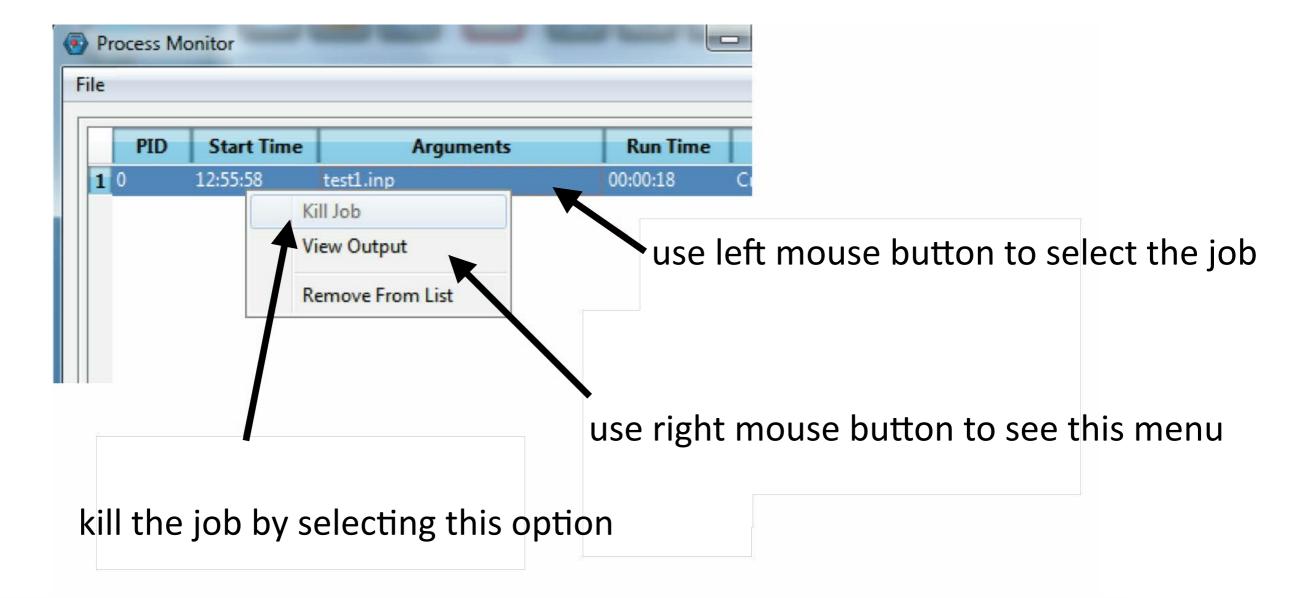
Check job status





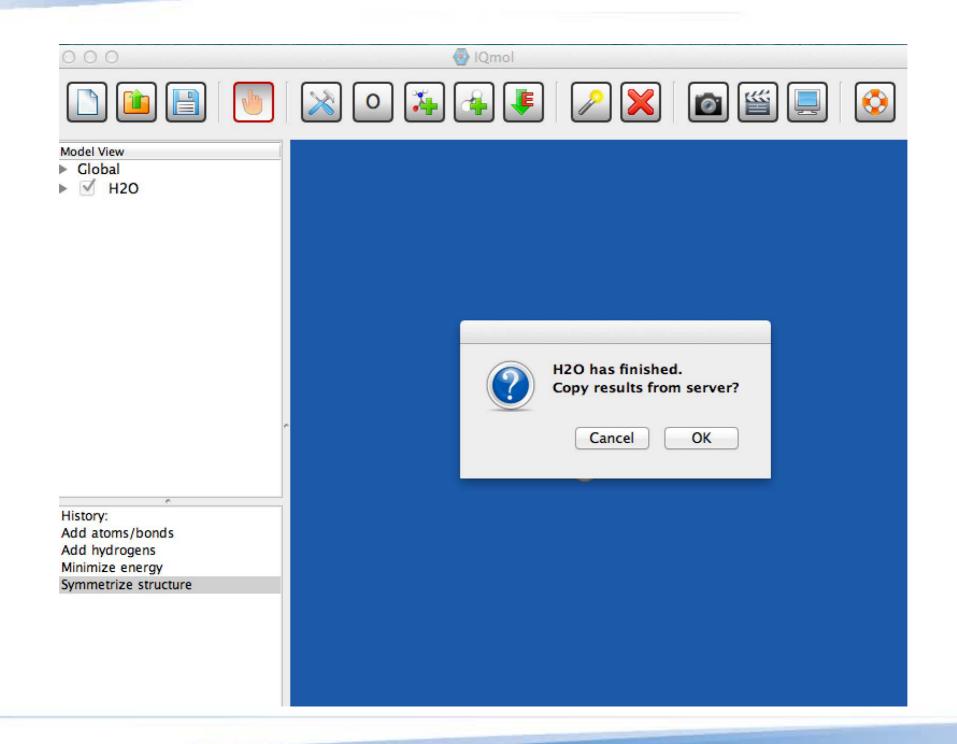
Check job status

Job status will be displayed in a new window:





Job is finished

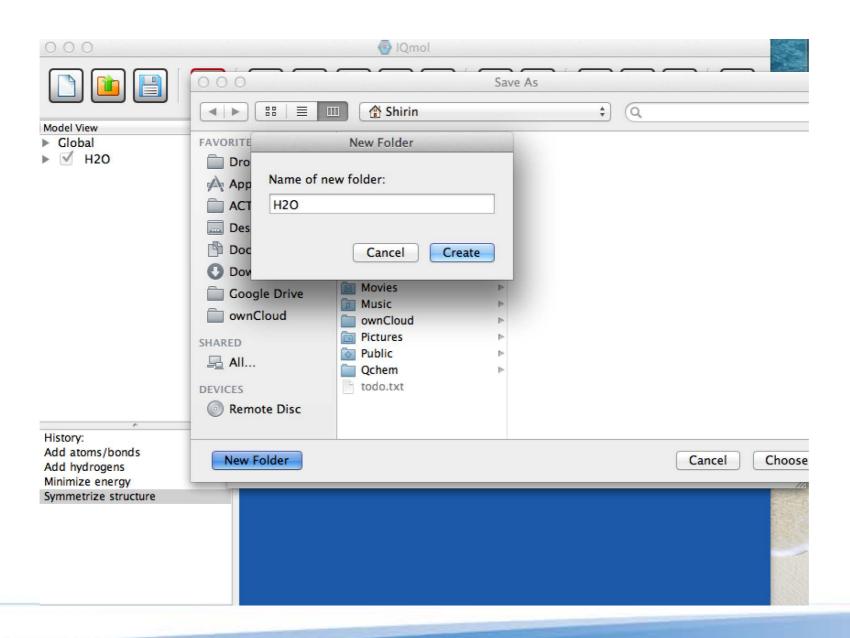




Copy files to your laptop

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!

