CHEM-E4110 - Quantum mechanics and Spectroscopy

Wihuri computing cluster

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Rules for using Wihuri

- 1. For the exercise sessions and related coursework, you will get a personal user account
- 2. You are only allowed to use your account until the end of the course
- 3. You are only allowed to carry out course-related work on the cluster
- 4. Giving the details of the user account to anyone else is strictly forbidden
- 5. Trying to install any software on the cluster is **strictly forbidden**
- 6. Trying to modify any files outside the home directory of your user account is strictly forbidden

Usage instructions for Wihuri

The address of the cluster is wihuri.pub.chemistrylab.aalto.fi

- On Linux computers, you can connect with ssh -I YOUR_USERNAME -X wihuri.pub.chemistrylab.aalto.fi
- On Windows computer, you must use an SSH client like PuTTY

For basic Linux usage, please see Google.

Important: All calculations need to be run using the queueing system! Let's see how it works.

Let us now assume that in the current working directory there is Orca input file h20.inp

- The job can be submitted to the queue with the command jsub orca h2o.inp
- You can check the status of the queue with the command **jstat**
- You can delete a job from the queue with the command jdel JOB_ID (JOB_ID comes from jstat)
- You can find the output from **h2o.oout**
- If your job runs into trouble, please see the output file and **h2o.batch-log** for error messages

Technical details (useful, but not necessary for running calculations)

- The cluster has four "nodes" (physically separate servers).
- Each node is equipped with two CPUs and in total 12 CPU cores.
- Never run Orca jobs with more than 12 CPUs during this course.
- Each node has 64 GB of RAM, meaning that jobs can be allocated max. 5 GB of RAM / CPU
- The amount of memory can be tuned with e.g. jsub -mem 2G orca h2o.inp
- The default is 1 GB / CPU, which should be enough for the calculations on this course