**Running Quantum Espresso H2O Example**

1. Log into your CHTC account:
   1. Follow instructions here:

<https://chtc.cs.wisc.edu/uw-research-computing/connecting>

1. Make and enter a working directory to run the example with commands ( replace USERNAME with your username ):

*cd /scratch/USERNAME*

*mkdir h2o\_example*

*cd h2o\_example*

1. Copy example files from group directory with command:

*cp* ***/****home/groups/mse\_course\_ping/examples/QE/input\_files/\* ./*

1. You can view the copied files with the command:

*ls*

You should see a list of files like:

**convert\_QE2XSF.py o\_pbe\_v1.2.uspp.F.UPF run\_h2o\_example.sh**

**wave1.in wave3.in wave5.in h\_pbe\_v1.4.uspp.F.UPF relax.in scf.in wave2.in wave4.in wave6.in**

1. You can then run the example by submitting a batch job to the SLURM scheduler with command:

*sbatch run\_h2o\_example.sh*

NOTE: Visit <https://slurm.schedmd.com> for more information on the SLURM Job Scheduling software.

1. To get the structure from the relaxation use this command to get ‘structure.xsf’ file:

*./convert\_QE2XSF.py*

NOTE: convert\_QE2XSF.py won’t work if you didn’t already set up your environment with instructions in “Setup\_CHTC\_Environment”

1. Structure You can then copy the output files to your local machine using the guide here: <https://chtc.cs.wisc.edu/uw-research-computing/transfer-files-computer>
2. You can visualize the output with visualization software:
   1. Online:
      1. Materials Cloud (<https://www.materialscloud.org/work/tools/qeinputgenerator> )
   2. Download and install:
      1. VESTA (<https://jp-minerals.org/vesta/en/> )
      2. XCrySden (<http://www.xcrysden.org> )