**WEEK 6 – Submitting calculations on a SCITAS cluster**

**Part 1. Useful information**

The clusters use slurm as scheduler, the following commands can be useful:

* sbatch is used to submit jobs
* squeue lists all jobs in the queue, the option -u <username> is particularly useful, as it lists only the jobs of the user username
* scontrol show jobid -dd <jobid> can be used to get detailed information about a job
* similarly, sstat -format=AveCPU,AvePages,AveRSS,AveVMSize,JobID -j <jobid> -allsteps prints some statistics for a job
* for finished jobs, you can find out more using:

sacct -j <jobid> -format=JobID,JobName,MaxRSS,Elapsed

sacct -u <username> -format=JobID,JobName,MaxRSS,Elapsed

* to cancel a job, you can use scancel <jobid>. And to cancel all jobs of user username, one can use scancel -u <username> or scancel -t PENDING -u <username> to cancel pending jobs or scancel -name myJobName to cancel jobs by name
* in some cases, it can also be useful to hold jobs. This can be accomplished with scontrol hold <jobid>. It can be released with scontrol release <jobid>

https://scitas.epfl.ch

https://slurm.schedmd.com/ quickstart.html

**What do you need to submit a calculation?**

You will need:

* your input file (we will adapt the ones you built so we can use another functional, I will give one as an example)
* a submission file (*e.g.* run.sh) that you can submit with sbatch run.sh
* other useful files: you can have the .xyz of your structure in the folder alongside with the submission and input file, so you can make a more organized input file (that way you can specify the structure file you want instead of copying and pasting the coordinates on the input file)
* if you are restarting a calculation, you will need the restart wavefunction (the extension of this file is .wfn)

**How to prepare your structure?**

If you are downloading it from a paper, the crystallographic information can be messy. If you have a .cif file, open it with a visualizer (like avogadro) and save as .xyz. Also take note on the crystal cell parameters (abc length and angles), you can find this information either on the visualizer or opening the file as a text.

To make it into a .cif again you can follow the steps detailed on the previous tutorials, from the .xyz you generated.

**Part 2. This week’s schedule**

We will run a single point (energy) calculation and learn about input and output files. While it is running, you can use the time reading about the keywords you can use in the input file on the cp2k input reference manual (<https://manual.cp2k.org/#gsc.tab=0>) and figure out what you can do with it. If we have time, you will also start with the optimization.

You will need to unzip this week’s folder and copy the run.sh and your input file to the supercomputer, for example:

scp run.sh <yourusername>@helvetios.epfl.ch:/scratch/<yourusername>

(you should run this on the terminal, making sure you are in the folder that has the input file; you can also get information about the path where you want to copy by accessing your account on the supercomputer and typing pwd)

You should edit the run.sh file (before running, you can do it on any text editor, for example by typing vi run.sh on the terminal), adding the information: name of the input file, name of the output file, your email and name of the job.

After you get the result, we can analyze the .out file:

Did the SCF converge?

What is the HOMO-LUMO gap?

What is the Fermi energy?