Instruction on how to access the supercomputer

Before the beginning of Lab 2, we want to check that you are able to log in to the `helvetios` supercomputer using the command ssh (secure shell) and run a simple calculation. Please perform the following steps:

1. **Install and connect to the EPFL VPN**. This is not required if you are connecting to the internet from within EPFL). This has to be done on your computer and not inside the VM. The instructions to install and use the EPFL VPN can be found here. This will allow you to connect to the internet as if you were inside EPFL, giving you access to the local network where the `helvetios` cluster is located
2. **Connect to the cluster**
    a. From within the VM (or using any SSH client, e.g. Putty on Windows)
    `ssh <USERNAME>@helvetios.hpc.epfl.ch`
    where you should replace `<USERNAME>` with your gaspar username (delete the `<>`'s!)
    b. If this is your first time connecting you might be prompted to add the server signature to the `known_hosts` by typing 'yes'.
    c. You will be prompted to enter your GASPAR password in order to complete the login
    d. If this doesn't work, please run this command with the `-v` option
    `ssh -v <USERNAME>@helvetios.hpc.epfl.ch`
    (the output of which will be needed for the google form below)
3. **Download and unzip the test files**
    a. Change into your scratch directory (`cd /scratch/<USERNAME>`)
    b. Run the command
    `wget 'https://docs.google.com/uc?export=download&id=1BSqhGeqo-uwlzgMrXG_Mf-b9Gyo8tpiL' -O mse468-helvetios-test.zip`
    This should download a zip called `mse468-helvetios-test.zip` to your current directory
    c. Unzip the archive via the command
    `unzip mse468-helvetios-test.zip`
    A folder of the same name should appear.
4. **Run the calculation**
    a. Change into the `mse468-helvetios-test/` subdirectory. You will see it contains an input file, a folder containing some pseudopotentials, and a script that we will use to submit calculations to the supercomputer.
    b. Submit the calculation to the supercomputer by running the command
    `sbatch submit.sh`
    This will submit your job to the supercomputer's queue, and will print to the screen:
    `Submitted batch job <job-number>`
    Note this job number down.
    c. Once there are available resources, the supercomputer will run your calculation. You can monitor the status of your job either using the command
    `sacct -j <job-number>`
    or
    `squeue -u <USERNAME>`
    d. Once your job is running (this should take less than a minute, but might take longer depending on how busy the supercomputer is), an output file `MgS_primitive.scf.out` will appear as well as a logfile called `slurm-<job number>.out`. The calculation itself will only take a couple of seconds. The job is complete if you open the output file and at the very end of the file there is a line that says `JOB DONE`.
5. **Verify the calculation**
    a. Note down the total energy that the calculation reports. You can get this easily via the command
    `grep ! MgS_primitive.scf.out`
6. **Complete this google form**. We will be in touch via email to address any issues before the labs begin