A few important Unix commands

You need to learn a few Unix commands in order to carry out the calculations in the course. Knowing how to use a Unix computer will also likely be beneficial in future scientific work. Many scientific programs are exclusively written for Unix computers and are used through the command-line interface (i.e. without a graphical user interface). Almost all scientific computer clusters use some type of Unix operating system, for example Linux. MaxOS X is a Unix based operating system. Both Linux and MacOS X have terminal windows where one can type in Unix commands and it is easy to connect to other Unix based computers, such as the computer cluster Elja. From a computer running the Windows operating system, you will need to install and use an SSH tool (see the guide for installing software for the course). Below is a summary of the most important commands.

A directory is analogous to a folder, it can contain several files. For example, it would make sense to make a directory for the files you create in this computational chemistry course. After logging in to Elja, type 'mkdir CompChem' to create a directory with the name CompChem. NOTE: Do not use Icelandic letters or spaces in names of directories and files. You can then enter the directory by typing 'cd CompChem'. In order to see what files are there, type 'ls'. The directory is empty at this point, but more and more files will be generated there as you carry out the work in this course. It is good practice to make a separate subdirectory for each of the exercises in the course. For example, make a subdirectory for testing called 'Lab1'. Eventually, you will create a tree of subdirectories. It is important to keep good order of the files you create and working with in the course.

You can see where in the directory tree you are located by typing 'pwd' which stands for 'print working directory'. The computer will then give you the path to the current directory. To move up in the directory tree type 'cd ..'.

You can create a new file with an editor, such as nano. Type 'nano newfile' to create a file called newfile. Any text you then write gets added to the file. To save what you have written on the disk, type 'Ctrl+O'. To exit nano, type 'Ctrl+X'.

You can change the name of a file using the 'mv' command, for example 'mv newfile oldfile'. You can also change the location at the same time, for example 'mv newfile ../oldfile' places the file with the new name at one level up in the

directory tree. You can also make a copy of the file with the 'cp' command. A file can be removed with the 'rm' command. It is important to clean up your directories regularly and delete unwanted files.

The contents of a file can be inspected quickly using either 'cat', 'less', or 'tail -n'. Try them all on files you have created. Make the file longer using nano and observe that 'cat' displays the whole file, while 'less' shows one page at a time. By hitting the space bar you get the next page. The 'tail -n' command shows the last n lines of the file.

Calculations on a computer cluster are handled by a queuing system. The one on Elja is called SLURM/PBS and a calculation is submitted to a queue typing 'sbatch jobscript.sh'. This will submit the script 'jobscript.sh' to a queue on Elja. The jobscript instructs the computer how to do the calculation. To check the status of all jobs submitted by a user, type 'squeue -u username', where the string 'username' is replaced by your user name.

To copy files from the cluster to your laptop, when you are working in a command line window on your laptop, type 'scp username@elja.hi.is:filename .' and the file will then be copied over to your current directory or folder on your computer (the last '.' in the command stands for current directory). The filename on Elja should contain the full path, i.e. name of directory and subdirectory, if applicable.

To quickly edit ORCA input ad output files it is recommended that you use a command line text editor. This is much quicker than moving a file over to your laptop and editing with an editor based on graphical user interface (such as Notepad or Textedit). The nano text editor is recommended. More advanced text editors include vim and emacs.

There are several tutorials available on the internet that explain how to use of the command line in Unix, for example:
`https://www.codecademy.com/courses/learn-the-command-line`
`http://www.ee.surrey.ac.uk/Teaching/Unix/`
`http://cli.learncodethehardway.org/book/`
`http://lifehacker.com/5633909/who-needs-a-mouse-learn-to-use-the-command-line-for-`