**GENERAL INSTRUCTIONS, LINUX Basics**

**1. LINUX Basics:**

A very brief reminder of useful linux commands:

* cp A B copies file A to file B.
* mv A B moves file A to file B.
* mkdir C creates a directory named C.
* ls C lists the names of the files and sub-directories contained in directory C
* vi A or gedit A are some of the many ways in which you can open the file A for reading and/or editing.
* Adding an ampersand & at the end of your command will make it run in the background, so that you can continue to issue other commands while the original one is still running.

Vi Editor Basic:

* vi A to open a file A for reading and/or editing.
* Shift+i to go into INSERT mode (Check for -- INSERT -- at the bottom of the file).
* Shift+r to go into REPLACE mode (Check for -- REPLACE -- at the bottom of the file).
* Esc to go into READ-ONLY mode
* To save your file: Esc (First go into READ-ONLY mode) and then :w (to save)
* To quit your file: Esc (First go into READ-ONLY mode) and then :q (to quit)

Remember: **don't overwrite** output files before you extract data from them!

**INSTRUCTIONS, EXERCISE 1**

Note that the following color code has been used in this instruction sheet:

Broad headings are in red.

File names are in magenta.

Phrases to be typed into the command line are in blue.

Input parameters are in dark green.

In this exercise, you will run a simple scf (self-consistent field) calculation on silicon.

* STEP 1: Go to the directory /home/username/Documents

The way to do this:

cd Documents

* STEP 2: Create a directory MS5023/exercise1 and MS5023/pseudos

mkdir MS5023

mkdir MS5023/exercise1

mkdir MS5023/pseudos

* STEP 3: Go to the directory /scratch/MS5023/exercise1

You will see the following files:

run.sh this is a sample SLURM job submission script

Si.sample.in this is a sample input file, for a primitive Si cell containing 2 atoms.

Si.pbe-rrkj.UPF this is a pseudo potential file.

Si\_icsd\_076268.cif Silicon structure data file in CIF format

* STEP 4: copy run.sh, Si.sample.in, Si.pbe-rrkj.UPF to your home working directory

cp run.sh Si.sample.in /home/username/Documents/MS5023/exercise1

cp Si.pbe-rrkj.UPF /home/username/Documents/MS5023/pseudos

* STEP 5: Go to your home working directory

cd /home/username/Documents/MS5023/exercise1

read the files run.sh and Si.sample.in using the text editor (VI)

run a scf calculation using job submission script run.sh:

sbatch run.sh

check if your job is running:

squeue -u username