Day 4 - Tuesday, 8th November , 2022
Introduction to Linux command line (CLI) Tools - Text Editing and Shell Scripting

In this exercise, the key commands you may need are as listed below.:
`grep` - search for pattern text in a file
`echo` - display lines of text or string
`cut` - cut sections of stings
`paste` - join files horizontally
`awk` - extracting data in columns

Some of the commands may require the use of **options** to attain the intended outcome. Look up the commands on the **man** pages to understand how to use respective options or refer to the slide. Tutors are also happy to help.

General preamble:
This set of exercises requires you to have a file "***N2H4_qe_output.txt"*** *and the zip file* ***nickel_Data.zip.*** Download(If you do not already have it in its original state) the files from the activity resource/materials pages(from previous Days' agenda) and have it placed in the respective directory of work. Having to move the data files to your preferred location will let you practise more on your command line navigation skill set.

To extract any ".**zip**" file, use: `unzip <file-name>`

Make a new directory in your `handson` directory(you created from your previous exercise) and call it "`shellscripts`"; For each of the exercises below, make a directory with the naming conventions "`exercise_<number>`". Eg "`exercise_1`" in "`shellscripts`". This will let you organise your work well so you can easily find respective files and/or directories when needed.

Exercise 1

> Write a script called `exercise_1.sh` that will utilise `grep` and `awk`, to extract only the **numeral value** of the Final energy in the data file "***N2H4_qe_output.txt"*** into a file called ***"final_energy.txt".***

Exercise 2

> Given a set of files being the output of multiple geometry optimization calculations to test for convergence by varying kinetic energy cut-off values(KECV), write a **bash script called** `exercise_2.sh` do what following:

> a. Extract the Final enthalpy values from those files((***Ni-<***KECV***>.out***)).

> b. Join or merge the data in the "*kine_ener.txt*" file and the extracted final energies accordingly to obtain an X-Y column data file called "***kiv_vrs_enthalpy.dat***".
> > - *Kinetic energy should be on the left and the Final **enthalpy** should be on the right.*

Exercise 3

Write a bash script called `exercise_3.sh` that will execute the activities in exercise 2 but with a 3rd column having the unit of the energy in eV. Unit of energy in the 2nd column is in Ryberg. The energy should be converted to **eV** during the awk operation to extract the final energy values and have it placed in a three(3) column file called "***final_ry_ev.dat***". *1 Ry = 13.605 **eV***

Basically, the file should have the following:
#Kinetic Energy Cut-off   #Final Energy in Ry #Final Energy in eV
You can give the headers any meaningful name that you want.