Day 3 - Thursday, 3rd November , 2022
Introduction to Linux command line (CLI) Tools.

In this exercise, the key commands you will 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

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 the file from the activity resource/materials page 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 skillset.

To extract the the zip file, use: `unzip <file-name>`

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

Exercise 1

Using `grep` and `awk`, 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 output of multiple geometry optimization calculations to test for convergence by varying kinetic energy cut-off values(KECV), extract the Final energies values from those files((***Ni-<***KECV***>.out***)).

A file, "*kine_ener.txt*", with a list of kinetic energy cut-off values has been provided. Join or merge the data in the "*kine_ener.txt*" 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

Stemming from exercise 2, the unit of the energy is in Ryberg. Convert it 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.