Day 2 - Thursday, 27th October, 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:
Make a new directory in your `handson` directory(you created from your previous exercise.)
and call it "`cmdtools`"; For each of the exercises below, make a directory called
exercise_<number>. Eg "`exercise_1`" in "`cmdtools`". This will let you organized your
work well so you can easily find respective files and/or directories when needed.

Exercise 1
1. Make a new directory in your `handson` directory(you created from your previous
    exercise.) and call it "`cmdtools`";
2. **echo** "Day 2 - CLI Tools" into file <`yourLastname_smr3821.txt`> and have it
    placed in the directory created from step 1 in this exercise."
    a. *hint*: At this point, you can either navigate into the target directory and
        execute this very step(2) or stay in the handson directory execute this step
        and move the resulting file into the target of concern.
    b. NB: if your handson directory was created well according to instructions from
        previous exercise, it should have the path '`/home/ictpuser/handson`'.

3. Use grep to get the occurrences of the word "final", ignoring case sensitivity, in the
    target file "**N2H4_qe_output.txt**" and inspect the output to know if there both
    uppercase and loser occurrences.
4. After inspections, use grep to the final string that has "energy" next to it and re-direct
    the output into a file called "final_energy.txt" .

Exercise 2 -

The file in the path `/etc/passwd` is a system configuration file that contains certain
important details. The structure of the information in the file is as follows:
 username, password denoted by x, user ID(UID), group ID, UserID info (GECOS), path to
home directory, Command/Shell.

Using `cut` and `grep`, get the **username** values into and file called "username.txt".
Using `cut` and `grep`, get the **UID** values into and file called "uid.txt"

Use `paste` to put them together in a single file called "**username_uid.txt**"

If it's done right, the file "**username_uid.txt"** should have a two columns of strings and integers that are supposed to be usernames and UIDs of users on the machine/computer you're using.
If you think you can use other cmd tools, besides cut and grep, to grab the usernames and UIDs from the `/etc/passwd` file, you can do so and share the idea.

username_uid.txt

```
systemd 104
george 105
apache 106
ictpuser 110
cups 999
avahi 1000
postfix 121
fwups 1001
```

Exercise 3 - Energy Minimization Inspection exercise

The file "**N2H4_qe_output.txt"** contains the output of a full geometry optimization calculation of the chemical system Ni-N_2H_4. The data consists of trajectories and accompanied energies from the cycle of calculations. Each cycle is denoted in the file by the string "**number of scf cycles**". The accompanied energy of each cycle is denoted by an exclamation mark, **!**.

Using `echo`, `grep` and `cut`, extract the enggies of the geometry optimization calculations along with the scf steps(or cycle counts) into a file "*ener_data.dat*" so we could plot and visualise to know if the energy of the system is really being minimised.

Data in "*ener_data.dat*" should have column labels: #steps   #energy
NB: Also pay attention that there may be a mismatch in the count of the steps vrs the extracted energies. Find a way to add the missing step(no of step)