Assignment 5

ESE 5023

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1.   More linux commands

1. 1 make a link

Pre-requests: ssh to Taiyi Frame and move to the root directory.

```
Last login: Wed Nov 24 20:12:10 on ttys000

The default interactive shell is now zsh.
To update your account to use zsh, please run `chsh -s /bin/zsh`.
For more details, please visit https://support.apple.com/kb/HT208050.
(base) Ziyans-MacBook-Pro:~ ziyanzhang$ ssh -l ese-zhangzy 172.18.6.175
ese-zhangzy@172.18.6.175's password:
Last login: Wed Nov 24 20:00:46 2021 from gpfsgui
Welcome to the SUSTech HPC
```

```
[ese-zhangzy@login01 ~]$ ls
data_demo  exam  hello.sh
[ese-zhangzy@login01 ~]$ ln -s data_demo data_demo_link
[ese-zhangzy@login01 ~]$ ls
data_demo  data_demo_link  exam  hello.sh
[ese-zhangzy@login01 ~]$
```

In the first question, I create a soft link with ln -s.

1.2 Echo

```
[ese-zhangzy@login01 ~]$ var=$(pwd)
[ese-zhangzy@login01 ~]$ echo $var
/work/ese-zhangzy
```

Firstly I propose a variable var to carry the pwd command, then echo the
executed command with echo $var.

1.3 Touch

```
[ese-zhangzy@login01 ~]$ cd data_demo/molecules/
[ese-zhangzy@login01 molecules]$ touch test.pdb
[ese-zhangzy@login01 molecules]$ ls -l
total 3
-rwxr-xr-x 1 ese-zhangzy ese-ouycc 1158 Nov 24 19:18 cubane.pdb
-rwxr-xr-x 1 ese-zhangzy ese-ouycc  622 Nov 24 19:18 ethane.pdb
-rwxr-xr-x 1 ese-zhangzy ese-ouycc  422 Nov 24 19:18 methane.pdb
-rwxr-xr-x 1 ese-zhangzy ese-ouycc 1828 Nov 24 19:18 octane.pdb
-rwxr-xr-x 1 ese-zhangzy ese-ouycc 1226 Nov 24 19:18 pentane.pdb
-rwxr-xr-x 1 ese-zhangzy ese-ouycc  825 Nov 24 19:18 propane.pdb
-rw-r--r-- 1 ese-zhangzy ese-ouycc    0 Nov 25 14:03 test.pdb
```

In this section, I first go to the target directory, then make an empty file through touch. At last, I use ls -l to examine the result.

1.4 Find and count

```
[ese-zhangzy@login01 data_demo]$ find data/elements -type f | wc -l
103
```

I use the method fine by type to get a list of files, then concatenate with word count by lines method to determine the number of qualified files.

1.5 Compare with diff

```
[ese-zhangzy@login01 data_demo]$ diff data/pdb/ethane.pdb data/pdb/ethanol.pdb
1,11c1,12
< COMPND      ETHANE
< AUTHOR      DAVE WOODCOCK  95 12 18
< ATOM      1  C           1      -0.752   0.001  -0.141  1.00  0.00
< ATOM      2  C           1       0.752  -0.001   0.141  1.00  0.00
< ATOM      3  H           1      -1.158   0.991   0.070  1.00  0.00
< ATOM      4  H           1      -1.240  -0.737   0.496  1.00  0.00
< ATOM      5  H           1      -0.924  -0.249  -1.188  1.00  0.00
< ATOM      6  H           1       1.158  -0.991  -0.070  1.00  0.00
< ATOM      7  H           1       0.924   0.249   1.188  1.00  0.00
< ATOM      8  H           1       1.240   0.737  -0.496  1.00  0.00
< TER       9               1
---
> COMPND      ETHANOL
> AUTHOR      DAVE WOODCOCK  96 01 03
> ATOM      1  C           1      -0.426  -0.115  -0.147  1.00  0.00
> ATOM      2  O           1      -0.599   1.244  -0.481  1.00  0.00
> ATOM      3  H           1      -0.750  -0.738  -0.981  1.00  0.00
> ATOM      4  H           1      -1.022  -0.351   0.735  1.00  0.00
> ATOM      5  H           1      -1.642   1.434  -0.689  1.00  0.00
> ATOM      6  C           1       1.047  -0.383   0.147  1.00  0.00
> ATOM      7  H           1       1.370   0.240   0.981  1.00  0.00
> ATOM      8  H           1       1.642  -0.147  -0.735  1.00  0.00
> ATOM      9  H           1       1.180  -1.434   0.405  1.00  0.00
> TER      10               1
```

1.6 Grep

```
[ese-zhangzy@login01 data_demo]$ grep -c 'But she' writing/data/LittleWomen.txt
15
```

The command stands for find and count the total line number of 'But she' inside the target file.

1.7 Disk Usage

```
[ese-zhangzy@login01 data_demo]$ du data
407     data/pdb
52      data/elements
1       data/animal-counts
719     data
```

Du command checks the disk usage.

1.8 Zip & Unzip

```
[ese-zhangzy@login01 data_demo]$ cp -r writing/ writing_new/
[ese-zhangzy@login01 data_demo]$ ls
creatures    data_demo_link   north-pacific-gyre   pizza.cfg   thesis          writing
data         molecules        notes                solar.pdf   thesis_backup   writing_new
```

Cp -r means copy the whole directory recursively,

```
[ese-zhangzy@login01 data_demo]$ zip -q -r writing_new.zip writing_new
[ese-zhangzy@login01 data_demo]$ ls
creatures        molecules             pizza.cfg   thesis_backup   writing_new.zip
data             north-pacific-gyre    solar.pdf   writing
data_demo_link   notes                 thesis      writing_new
```

Zip -q -r means zip without showing the process, and zip the directory

recursively.

```
[ese-zhangzy@login01 data_demo]$ unzip writing_new.zip
Archive:  writing_new.zip
replace writing_new/haiku.txt? [y]es, [n]o, [A]ll, [N]one, [r]ename: A
  inflating: writing_new/haiku.txt
 extracting: writing_new/tools/stats
 extracting: writing_new/tools/old/oldtool
  inflating: writing_new/tools/format
  inflating: writing_new/data/one.txt
  inflating: writing_new/data/LittleWomen.txt
  inflating: writing_new/data/two.txt
 extracting: writing_new/thesis/empty-draft.md
[ese-zhangzy@login01 data_demo]$ ls
creatures        molecules             pizza.cfg   thesis_backup   writing_new.zip
data             north-pacific-gyre    solar.pdf   writing
data_demo_link   notes                 thesis      writing_new
```

Upzip the file with replacing the duplicate one.

1.9 Chmod

```
[ese-zhangzy@login01 data_demo]$ chmod 750 writing_new
[ese-zhangzy@login01 data_demo]$ ls -l
total 646
drwxr-xr-x 2 ese-zhangzy ese-ouycc    4096 Nov 24 19:18 creatures
drwxr-xr-x 5 ese-zhangzy ese-ouycc    4096 Nov 24 19:18 data
lrwxrwxrwx 1 ese-zhangzy ese-ouycc      14 Nov 25 13:59 data_demo_link -> data_demo_link
drwxr-xr-x 2 ese-zhangzy ese-ouycc    4096 Nov 25 14:03 molecules
drwxr-xr-x 3 ese-zhangzy ese-ouycc    4096 Nov 24 19:18 north-pacific-gyre
-rwxr-xr-x 1 ese-zhangzy ese-ouycc      69 Nov 24 19:18 notes
-rwxr-xr-x 1 ese-zhangzy ese-ouycc      32 Nov 24 19:18 pizza.cfg
-rwxr-xr-x 1 ese-zhangzy ese-ouycc   21583 Nov 24 19:18 solar.pdf
drwxr-xr-x 3 ese-zhangzy ese-ouycc    4096 Nov 24 20:02 thesis
drwxr-xr-x 3 ese-zhangzy ese-ouycc    4096 Nov 24 20:02 thesis_backup
drwxr-xr-x 5 ese-zhangzy ese-ouycc    4096 Nov 24 19:18 writing
drwxr-x--- 5 ese-zhangzy ese-ouycc    4096 Nov 25 14:23 writing_new
-rw-r--r-- 1 ese-zhangzy ese-ouycc  422584 Nov 25 14:22 writing_new.zip
```

750 stands for all rights for the owner, read and execute only for group users,

no access for other users.

1.10 History

```
[ese-zhangzy@login01 data_demo]$ history 10
  173  ls
  174  unzip writing_new.zip
  175  ls
  176  chmod writing_new 750
  177  chmod 750 writing_new
  178  ls -l
  179  history -10
  180  history -N 10
  181  history -n 10
  182  history 10
```

2. BASH Coding

Explanation: Use cat to create a BASH file, iterate every file with expansion '.pdb' with command find, then output the count of bytes through command wc -c.

```
[ese-zhangzy@login01 ~]$ cat > echo_size.sh
#!/bin/bash
for file in $(find data_demo/data/pdb/ -name '*.pdb')
do
wc -c $file
done
^C
[ese-zhangzy@login01 ~]$ sh echo_size.sh
11193 data_demo/data/pdb/lanoxin.pdb
490 data_demo/data/pdb/methanol.pdb
1694 data_demo/data/pdb/citronellal.pdb
2729 data_demo/data/pdb/norethindrone.pdb
4209 data_demo/data/pdb/heme.pdb
2123 data_demo/data/pdb/mustard.pdb
306 data_demo/data/pdb/ammonia.pdb
1444 data_demo/data/pdb/ascorbic-acid.pdb
1064 data_demo/data/pdb/lactic-acid.pdb
422 data_demo/data/pdb/methane.pdb
2288 data_demo/data/pdb/morphine.pdb
2287 data_demo/data/pdb/piperine.pdb
2562 data_demo/data/pdb/maltose.pdb
2787 data_demo/data/pdb/testosterone.pdb
2196 data_demo/data/pdb/thiamine.pdb
3303 data_demo/data/pdb/quinine.pdb
2103 data_demo/data/pdb/tyrian-purple.pdb
2395 data_demo/data/pdb/tuberin.pdb
1090 data_demo/data/pdb/cinnamaldehyde.pdb
2894 data_demo/data/pdb/vitamin-a.pdb
2396 data_demo/data/pdb/ethylcyclohexane.pdb
2675 data_demo/data/pdb/strychnine.pdb
2562 data_demo/data/pdb/sucrose.pdb
1226 data_demo/data/pdb/pentane.pdb
1680 data_demo/data/pdb/nerol.pdb
423 data_demo/data/pdb/vinyl-chloride.pdb
1830 data_demo/data/pdb/camphene.pdb
1516 data_demo/data/pdb/aldrin.pdb
1158 data_demo/data/pdb/cubane.pdb
690 data_demo/data/pdb/ethanol.pdb
5049 data_demo/data/pdb/cholesterol.pdb
895 data_demo/data/pdb/cyclobutane.pdb
1508 data_demo/data/pdb/tnt.pdb
1361 data_demo/data/pdb/vanillin.pdb
1869 data_demo/data/pdb/mint.pdb
1256 data_demo/data/pdb/pyridoxal.pdb
622 data_demo/data/pdb/ethane.pdb
1030 data_demo/data/pdb/benzaldehyde.pdb
3395 data_demo/data/pdb/lsd.pdb
825 data_demo/data/pdb/propane.pdb
1384 data_demo/data/pdb/cyclohexanol.pdb
765 data_demo/data/pdb/glycol.pdb
2452 data_demo/data/pdb/codeine.pdb
1159 data_demo/data/pdb/styrene.pdb
695 data_demo/data/pdb/cyclopropane.pdb
2164 data_demo/data/pdb/menthol.pdb
1828 data_demo/data/pdb/octane.pdb
2562 data_demo/data/pdb/lactose.pdb
[ese-zhangzy@login01 ~]$ ▮
```