Assignment 05

1. More Linux Commands

   1.1

   ```
   [ese-zhangk@login03 ~]$ ln -s data_demo data_demo_link
   ```

   ```
   [ese-zhangk@login03 ~]$ ls
   data_demo  data_demo_link  exam  mpi_demo
   ```

   1.2

   ```
   [ese-zhangk@login03 ~]$ echo $HOME
   /work/ese-zhangk
   ```

   1.3

   ```
   [ese-zhangk@login03 molecules]$ touch test.pdb
   ```

   ```
   [ese-zhangk@login03 molecules]$ ls
   cubane.pdb  methane.pdb  pentane.pdb  test.pdb
   ```

   1.4

   ```
   [ese-zhangk@login03 ~]$ find data_demo/data/elements/ -type f | wc -w
   103
   ```

   1.5

   ```
   [ese-zhangk@login03 ~]$ diff data_demo/data/pdb/ethane.pdb data_demo/data/pdb/et
   hanol.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

   ```
   [ese-zhangk@login03 ~]$ grep But\ she data_demo/writing/data/LittleWomen.txt | w
   c -l
   15
   ```

   1.7

   ```
   [ese-zhangk@login03 ~]$ du -sh data_demo/data/
   721K    data_demo/data/
   ```

   1.8

```
[ese-zhangk@login03 data_demo]$ cd ..
[ese-zhangk@login03 ~]$ cp -r data_demo/writing/ data_demo/writing_new/
[ese-zhangk@login03 ~]$ zip -r writing_zip.zip data_demo/writing_new/
  adding: data_demo/writing_new/ (stored 0%)
  adding: data_demo/writing_new/haiku.txt (deflated 29%)
  adding: data_demo/writing_new/tools/ (stored 0%)
  adding: data_demo/writing_new/tools/stats (stored 0%)
  adding: data_demo/writing_new/tools/old/ (stored 0%)
  adding: data_demo/writing_new/tools/old/oldtool (stored 0%)
  adding: data_demo/writing_new/tools/format (deflated 13%)
  adding: data_demo/writing_new/data/ (stored 0%)
  adding: data_demo/writing_new/data/one.txt (deflated 53%)
  adding: data_demo/writing_new/data/LittleWomen.txt (deflated 61%)
  adding: data_demo/writing_new/data/two.txt (deflated 59%)
  adding: data_demo/writing_new/thesis/ (stored 0%)
  adding: data_demo/writing_new/thesis/empty-draft.md (stored 0%)
[ese-zhangk@login03 ~]$ ls
data_demo    data_demo_link   exam   mpi_demo   writing_zip.zip
[ese-zhangk@login03 ~]$ unzip writing_zip.zip
Archive:   writing_zip.zip
replace data_demo/writing_new/haiku.txt? [y]es, [n]o, [A]ll, [N]one, [r]ename: y
  inflating: data_demo/writing_new/haiku.txt
replace data_demo/writing_new/tools/stats? [y]es, [n]o, [A]ll, [N]one, [r]ename:
 y
```

```
 extracting: data_demo/writing_new/tools/stats
replace data_demo/writing_new/tools/old/oldtool? [y]es, [n]o, [A]ll, [N]one, [r]
ename: y
 extracting: data_demo/writing_new/tools/old/oldtool
replace data_demo/writing_new/tools/format? [y]es, [n]o, [A]ll, [N]one, [r]ename
: y
  inflating: data_demo/writing_new/tools/format
replace data_demo/writing_new/data/one.txt? [y]es, [n]o, [A]ll, [N]one, [r]ename
: y
  inflating: data_demo/writing_new/data/one.txt
replace data_demo/writing_new/data/LittleWomen.txt? [y]es, [n]o, [A]ll, [N]one,
[r]ename: y
  inflating: data_demo/writing_new/data/LittleWomen.txt
replace data_demo/writing_new/data/two.txt? [y]es, [n]o, [A]ll, [N]one, [r]ename
: y
  inflating: data_demo/writing_new/data/two.txt
replace data_demo/writing_new/thesis/empty-draft.md? [y]es, [n]o, [A]ll, [N]one,
 [r]ename: y
 extracting: data_demo/writing_new/thesis/empty-draft.md
[ese-zhangk@login03 ~]$ y
bash: y: command not found...
```

1.9

```
[ese-zhangk@login03 ~]$ chmod 750 data_demo/writing_new/
[ese-zhangk@login03 ~]$ cd data_demo
[ese-zhangk@login03 data_demo]$ ll
total 134
drwxr-xr-x 2 ese-zhangk ese-ouycc  4096 Dec  7 13:43 creatures
drwxr-xr-x 5 ese-zhangk ese-ouycc  4096 Dec  7 13:43 data
-rw-r--r-- 1 ese-zhangk ese-ouycc   637 Dec  7 13:43 log1
-rw-r--r-- 1 ese-zhangk ese-ouycc  1274 Dec  7 13:43 log2
drwxr-xr-x 2 ese-zhangk ese-ouycc  4096 Dec  7 13:43 molecules
drwxr-xr-x 3 ese-zhangk ese-ouycc  4096 Dec  7 13:43 north-pacific-gyre
-rwxr-xr-x 1 ese-zhangk ese-ouycc    76 Dec  7 13:43 notes
-rwxr-xr-x 1 ese-zhangk ese-ouycc    32 Dec  7 13:43 pizza.cfg
-rwxr-xr-x 1 ese-zhangk ese-ouycc 21583 Dec  7 13:43 solar.pdf
-rw-r--r-- 1 ese-zhangk ese-ouycc    20 Dec  7 13:43 temp
drwxr-xr-x 5 ese-zhangk ese-ouycc  4096 Dec  7 13:43 writing
drwxr-x--- 5 ese-zhangk ese-ouycc  4096 Dec  7 14:31 writing_new
```

1.10

```
[ese-zhangk@login03 data_demo]$ history 10
  312  chmod 750 data_demo/writing_new/
  313  cd data_demo/writing_new/
  314  ll
  315  cd ..
  316  ll
  317  cd ..
  318  cd data_demo
  319  ll
  320  history -10
  321  history 10
```

2. BASH for Loop

```
  GNU nano 2.3.1                 File: pri.sh                                    ^

for i in data_demo/data/pdb/*.pdb
do
    du -b $i
done












                            [ Read 4 lines ]
^G Get Help    ^O WriteOut   ^R Read File  ^Y Prev Page  ^K Cut Text   ^C Cur Pos
^X Exit        ^J Justify    ^W Where Is   ^V Next Page  ^U UnCut Text ^T To Spell  v
```

```
[ese-zhangk@login03 ~]$ nano pri.sh                                             ^
[ese-zhangk@login03 ~]$ bash pri.sh
1516    data_demo/data/pdb/aldrin.pdb
306     data_demo/data/pdb/ammonia.pdb
1444    data_demo/data/pdb/ascorbic-acid.pdb
1030    data_demo/data/pdb/benzaldehyde.pdb
1830    data_demo/data/pdb/camphene.pdb
5049    data_demo/data/pdb/cholesterol.pdb
1090    data_demo/data/pdb/cinnamaldehyde.pdb
1694    data_demo/data/pdb/citronellal.pdb
2452    data_demo/data/pdb/codeine.pdb
1158    data_demo/data/pdb/cubane.pdb
895     data_demo/data/pdb/cyclobutane.pdb
1384    data_demo/data/pdb/cyclohexanol.pdb
695     data_demo/data/pdb/cyclopropane.pdb
622     data_demo/data/pdb/ethane.pdb
690     data_demo/data/pdb/ethanol.pdb
2396    data_demo/data/pdb/ethylcyclohexane.pdb
765     data_demo/data/pdb/glycol.pdb
4209    data_demo/data/pdb/heme.pdb
1064    data_demo/data/pdb/lactic-acid.pdb
2562    data_demo/data/pdb/lactose.pdb
11193   data_demo/data/pdb/lanoxin.pdb
3395    data_demo/data/pdb/lsd.pdb                                              v
```

```
2562    data_demo/data/pdb/maltose.pdb
2164    data_demo/data/pdb/menthol.pdb
422     data_demo/data/pdb/methane.pdb
490     data_demo/data/pdb/methanol.pdb
1869    data_demo/data/pdb/mint.pdb
2288    data_demo/data/pdb/morphine.pdb
2123    data_demo/data/pdb/mustard.pdb
1680    data_demo/data/pdb/nerol.pdb
2729    data_demo/data/pdb/norethindrone.pdb
1828    data_demo/data/pdb/octane.pdb
1226    data_demo/data/pdb/pentane.pdb
2287    data_demo/data/pdb/piperine.pdb
825     data_demo/data/pdb/propane.pdb
1256    data_demo/data/pdb/pyridoxal.pdb
3303    data_demo/data/pdb/quinine.pdb
2675    data_demo/data/pdb/strychnine.pdb
1159    data_demo/data/pdb/styrene.pdb
2562    data_demo/data/pdb/sucrose.pdb
2787    data_demo/data/pdb/testosterone.pdb
2196    data_demo/data/pdb/thiamine.pdb
1508    data_demo/data/pdb/tnt.pdb
2395    data_demo/data/pdb/tuberin.pdb
2103    data_demo/data/pdb/tyrian-purple.pdb
1361    data_demo/data/pdb/vanillin.pdb
423     data_demo/data/pdb/vinyl-chloride.pdb
2894    data_demo/data/pdb/vitamin-a.pdb
```