

ESE5023 Assignment 05 Report

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1. More Linux Commands

1.1 [2 points] Make a link called data_demo_link to data_demo folder using ln.

```
ln -s data_demo/ data_demo_link
```

```
[ese-lijy@login03 ~]$ ln -s data_demo/ data_demo_link
[ese-lijy@login03 ~]$ ll
total 6
drwxr-xr-x 7 ese-lijy ese-ouycc 4096 Dec  3 16:16 data_demo
lrwxrwxrwx 1 ese-lijy ese-ouycc  10 Dec  8 01:25 data_demo_link -> data_demo/
-rw-r--r-- 1 ese-lijy ese-ouycc   0 Dec  1 20:27 err.log
-rw-r--r-- 1 ese-lijy ese-ouycc   0 Dec  1 20:44 err_t2.log
drwxr-xr-x 2 ese-lijy ese-ouycc 4096 Nov  2 18:48 exam
-rw-r--r-- 1 ese-lijy ese-ouycc 1818 Dec  1 20:27 job.log
-rw-r--r-- 1 ese-lijy ese-ouycc  384 Dec  1 19:56 job.lsf
-rw-r--r-- 1 ese-lijy ese-ouycc 1823 Dec  1 20:44 job_t2.log
-rw-r--r-- 1 ese-lijy ese-ouycc  389 Dec  1 20:28 jobt2.lsf
drwxr-xr-x 2 ese-lijy ese-ouycc 4096 Dec  3 17:55 mpi_demo
-rw-r--r-- 1 ese-lijy ese-ouycc  45 Dec  1 20:27 result.log
-rw-r--r-- 1 ese-lijy ese-ouycc  50 Dec  1 20:44 result_t2.log
-rw-r--r-- 1 ese-lijy ese-ouycc 206 Dec  1 20:30 t2.py
-rw-r--r-- 1 ese-lijy ese-ouycc 222 Dec  1 19:49 test.py
```

1.2 [2 points] Print your home directory using echo.

```
echo $HOME
```

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

1.3 [2 points] Go to data_demo/molecules/, make an empty file test.pdb with touch.

```
cd data_demo/molecules/
touch test.pdb
```

```
[ese-lijy@login03 ~]$ cd data_demo/molecules/
[ese-lijy@login03 molecules]$ touch test.pdb
[ese-lijy@login03 molecules]$ ls
cubane.pdb ethane.pdb methane.pdb octane.pdb pentane.pdb propane.pdb test.pdb
[ese-lijy@login03 molecules]$
```

1.4 [3 points] Find how many files in data_demo/data/elements/ using find.

```
find ./data_demo/data/elements/ -type f | wc -l
```

```
[ese-lijy@login03 ~]$ find ./data_demo/data/elements/ -type f | wc -l
103
[ese-lijy@login03 ~]$
```

1.5 [2 points] Compare data_demo/data/pdb/ethane.pdb and data_demo/data/pdb/ethanol.pdb with diff.

```
diff data_demo/data/pdb/ethane.pdb data_demo/data/pdb/ethanol.pdb
```

```
[ese-lijy@login03 ~]$ diff data_demo/data/pdb/ethane.pdb data_demo/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
---
> 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
[ese-lijy@login03 ~]$
```

1.6 [3 points] Count how many But she string appears in data_demo/writing/data/LittleWomen.txt with grep.

```
cat data_demo/writing/data/LittleWomen.txt | grep "But she" | wc -l
```

```
[ese-lijy@login03 ~]$ cat data_demo/writing/data/LittleWomen.txt | grep "But she" | wc -l
15
[ese-lijy@login03 ~]$
```

1.7 [2 points] Check the total file size of the data_demo/data/ folder using du.

```
du ./data_demo/data/ -hc
```

```
[ese-lijy@login03 ~]$ du ./data_demo/data/ -hc
408K    ./data_demo/data/pdb
52K     ./data_demo/data/elements
1.0K    ./data_demo/data/animal-counts
720K    ./data_demo/data/
720K    total
[ese-lijy@login03 ~]$
```

1.8 [3 points] Copy the data_demo/writing/ folder to data_demo/writing_new/, compress data_demo/writing_new/ using zip, and decompress the .zip file with unzip.

```
cd data_demo
cp writing/ writing_new/ -r
zip -r writing_new.zip ./writing_new/
unzip writing_new.zip -d unzip
```

```
[ese-lijy@login03 ~]$ cd data_demo
[ese-lijy@login03 data_demo]$ cp writing/ writing_new/ -r
[ese-lijy@login03 data_demo]$ ls writing_new/
data  haiku.txt  thesis  tools
[ese-lijy@login03 data_demo]$ zip -r writing_new.zip ./writing_new/
adding: writing_new/ (stored 0%)
adding: writing_new/haiku.txt (deflated 29%)
adding: writing_new/tools/ (stored 0%)
adding: writing_new/tools/stats (stored 0%)
adding: writing_new/tools/old/ (stored 0%)
adding: writing_new/tools/old/oldtool (stored 0%)
adding: writing_new/tools/format (deflated 13%)
adding: writing_new/data/ (stored 0%)
adding: writing_new/data/one.txt (deflated 53%)
adding: writing_new/data/LittleWomen.txt (deflated 61%)
adding: writing_new/data/two.txt (deflated 59%)
adding: writing_new/thesis/ (stored 0%)
adding: writing_new/thesis/empty-draft.md (stored 0%)
[ese-lijy@login03 data_demo]$ ls
creatures  data  log1  log2  molecules  north-pacific-gyre  notes  pizza.cfg  solar.pdf  writing  writing_new  writing_new.zip
[ese-lijy@login03 data_demo]$ unzip writing_new.zip -d unzip
Archive:  writing_new.zip
  creating: unzip/writing_new/
  inflating: unzip/writing_new/haiku.txt
  creating: unzip/writing_new/tools/
 extracting: unzip/writing_new/tools/stats
  creating: unzip/writing_new/tools/old/
 extracting: unzip/writing_new/tools/old/oldtool
  inflating: unzip/writing_new/tools/format
  creating: unzip/writing_new/data/
  inflating: unzip/writing_new/data/one.txt
  inflating: unzip/writing_new/data/LittleWomen.txt
  inflating: unzip/writing_new/data/two.txt
  creating: unzip/writing_new/thesis/
 extracting: unzip/writing_new/thesis/empty-draft.md
[ese-lijy@login03 data_demo]$ ls unzip/
writing_new
[ese-lijy@login03 data_demo]$ ls unzip/writing_new/
data  haiku.txt  thesis  tools
[ese-lijy@login03 data_demo]$
```

1.9 [3 points] Change the file permissions flags on writing_new to drwxr-x--- using chmod.

```
chmod 750 writing_new
```

```
[ese-lijy@login03 data_demo]$ ll
total 646
drwxr-xr-x 2 ese-lijy ese-ouycc 4096 Nov 24 19:21 creatures
drwxr-xr-x 5 ese-lijy ese-ouycc 4096 Dec 1 20:31 data
-rw-r--r-- 1 ese-lijy ese-ouycc 120 Dec 3 16:16 log1
-rw-r--r-- 1 ese-lijy ese-ouycc 120 Dec 3 16:16 log2
drwxr-xr-x 2 ese-lijy ese-ouycc 4096 Dec 8 01:32 molecules
drwxr-xr-x 3 ese-lijy ese-ouycc 4096 Nov 24 19:21 north-pacific-gyre
-rwxr-xr-x 1 ese-lijy ese-ouycc 69 Nov 24 19:21 notes
-rwxr-xr-x 1 ese-lijy ese-ouycc 32 Nov 24 19:21 pizza.cfg
-rwxr-xr-x 1 ese-lijy ese-ouycc 21583 Nov 24 19:21 solar.pdf
drwxr-xr-x 3 ese-lijy ese-ouycc 4096 Dec 8 02:04 unzip
drwxr-xr-x 5 ese-lijy ese-ouycc 4096 Nov 24 19:21 writing
drwxr-xr-x 5 ese-lijy ese-ouycc 4096 Dec 8 02:00 writing_new
-rw-r--r-- 1 ese-lijy ese-ouycc 422584 Dec 8 02:02 writing_new.zip
[ese-lijy@login03 data_demo]$ chmod 750 writing_new
[ese-lijy@login03 data_demo]$ ll
total 646
drwxr-xr-x 2 ese-lijy ese-ouycc 4096 Nov 24 19:21 creatures
drwxr-xr-x 5 ese-lijy ese-ouycc 4096 Dec 1 20:31 data
-rw-r--r-- 1 ese-lijy ese-ouycc 120 Dec 3 16:16 log1
-rw-r--r-- 1 ese-lijy ese-ouycc 120 Dec 3 16:16 log2
drwxr-xr-x 2 ese-lijy ese-ouycc 4096 Dec 8 01:32 molecules
drwxr-xr-x 3 ese-lijy ese-ouycc 4096 Nov 24 19:21 north-pacific-gyre
-rwxr-xr-x 1 ese-lijy ese-ouycc 69 Nov 24 19:21 notes
-rwxr-xr-x 1 ese-lijy ese-ouycc 32 Nov 24 19:21 pizza.cfg
-rwxr-xr-x 1 ese-lijy ese-ouycc 21583 Nov 24 19:21 solar.pdf
drwxr-xr-x 3 ese-lijy ese-ouycc 4096 Dec 8 02:04 unzip
drwxr-xr-x 5 ese-lijy ese-ouycc 4096 Nov 24 19:21 writing
drwxr-xr-x 5 ese-lijy ese-ouycc 4096 Dec 8 02:00 writing_new
-rw-r--r-- 1 ese-lijy ese-ouycc 422584 Dec 8 02:02 writing_new.zip
[ese-lijy@login03 data_demo]$
```

1.10 [3 points] Print the last 10 commands you made using history.

```
history | tail -n 10
```

```
[ese-lijy@login03 data_demo]$ history | tail -n 10
364 zip -r writing_new.zip ./writing_new/
365 ls
366 unzip writing_new.zip -d unzip
367 ls unzip/
368 ls unzip/writing_new/
369 ll
370 chmod 750 writing_new
371 ll
372 history
373 history | tail -n 10
[ese-lijy@login03 data_demo]$
```

2. BASH for Loop

```
nano pdb_size.sh
```

输入脚本，并保存文件:

```
#!/bin/bash
```

```
for pdb in $(du -b ~/data_demo/data/pdb/*.pdb)
do
    echo $pdb
done
```

```
chmod 750 pdb_size.sh
./pdb_size.sh
```

```
[ese-lijy@login03 ~]$ ./pdb_size.sh
1516
/work/ese-lijy/data_demo/data/pdb/aldrin.pdb
306
/work/ese-lijy/data_demo/data/pdb/ammonia.pdb
1444
/work/ese-lijy/data_demo/data/pdb/ascorbic-acid.pdb
1030
/work/ese-lijy/data_demo/data/pdb/benzaldehyde.pdb
1830
/work/ese-lijy/data_demo/data/pdb/camphene.pdb
5049
/work/ese-lijy/data_demo/data/pdb/cholesterol.pdb
1090
/work/ese-lijy/data_demo/data/pdb/cinnamaldehyde.pdb
1694
/work/ese-lijy/data_demo/data/pdb/citronellal.pdb
2452
/work/ese-lijy/data_demo/data/pdb/codeine.pdb
1158
/work/ese-lijy/data_demo/data/pdb/cubane.pdb
895
/work/ese-lijy/data_demo/data/pdb/cyclobutane.pdb
1384
/work/ese-lijy/data_demo/data/pdb/cyclohexanol.pdb
695
/work/ese-lijy/data_demo/data/pdb/cyclopropane.pdb
622
/work/ese-lijy/data_demo/data/pdb/ethane.pdb
690
/work/ese-lijy/data_demo/data/pdb/ethanol.pdb
2396
/work/ese-lijy/data_demo/data/pdb/ethylcyclohexane.pdb
765
/work/ese-lijy/data_demo/data/pdb/glycol.pdb
4209
/work/ese-lijy/data_demo/data/pdb/heme.pdb
1064
/work/ese-lijy/data_demo/data/pdb/lactic-acid.pdb
2562
/work/ese-lijy/data_demo/data/pdb/lactose.pdb
11193
/work/ese-lijy/data_demo/data/pdb/lanoxin.pdb
3395
/work/ese-lijy/data_demo/data/pdb/lsd.pdb
2562
/work/ese-lijy/data_demo/data/pdb/maltose.pdb
2164
/work/ese-lijy/data_demo/data/pdb/menthol.pdb
422
/work/ese-lijy/data_demo/data/pdb/methane.pdb
490
/work/ese-lijy/data_demo/data/pdb/methanol.pdb
1869
/work/ese-lijy/data_demo/data/pdb/mint.pdb
2288
/work/ese-lijy/data_demo/data/pdb/morphine.pdb
2123
/work/ese-lijy/data_demo/data/pdb/mustard.pdb
1680
/work/ese-lijy/data_demo/data/pdb/nerol.pdb
2729
/work/ese-lijy/data_demo/data/pdb/norethindrone.pdb
1828
/work/ese-lijy/data_demo/data/pdb/octane.pdb
1226
```

```
/work/ese-lijy/data_demo/data/pdb/pentane.pdb
2287
/work/ese-lijy/data_demo/data/pdb/piperine.pdb
825
/work/ese-lijy/data_demo/data/pdb/propane.pdb
1256
/work/ese-lijy/data_demo/data/pdb/pyridoxal.pdb
3303
/work/ese-lijy/data_demo/data/pdb/quinine.pdb
2675
/work/ese-lijy/data_demo/data/pdb/strychnine.pdb
1159
/work/ese-lijy/data_demo/data/pdb/styrene.pdb
2562
/work/ese-lijy/data_demo/data/pdb/sucrose.pdb
2787
/work/ese-lijy/data_demo/data/pdb/testosterone.pdb
2196
/work/ese-lijy/data_demo/data/pdb/thiamine.pdb
1508
/work/ese-lijy/data_demo/data/pdb/tnt.pdb
2395
/work/ese-lijy/data_demo/data/pdb/tuberin.pdb
2103
/work/ese-lijy/data_demo/data/pdb/tyrian-purple.pdb
1361
/work/ese-lijy/data_demo/data/pdb/vanillin.pdb
423
/work/ese-lijy/data_demo/data/pdb/vinyl-chloride.pdb
2894
/work/ese-lijy/data_demo/data/pdb/vitamin-a.pdb
[ese-lijy@login03 ~]$ █
```