

PS5

1. More Linux Commands

1.1 Make a link called data_demo_link to data_demo folder using ln.

```
[ese-wangyy@login02 ~]$ ln -s data_demo data_demo_link
[ese-wangyy@login02 ~]$ ll
total 4
drwxr-xr-x 8 ese-wangyy ese-ouycc 4096 Dec  3 16:41 data_demo
lrwxrwxrwx 1 ese-wangyy ese-ouycc    9 Dec  3 19:02 data_demo_link -> data_demo
drwxr-xr-x 2 ese-wangyy ese-ouycc 4096 Nov  2 18:47 exam
-rwxr-x--- 1 ese-wangyy ese-ouycc  50 Dec  1 20:28 ll2.sh
-rwxr-x--- 1 ese-wangyy ese-ouycc  31 Dec  1 20:25 logest.sh
drwxr-xr-x 2 ese-wangyy ese-ouycc 4096 Dec  3 17:57 mpi_demo
drwxr-xr-x 2 ese-wangyy ese-ouycc 4096 Nov 24 19:57 test
```

1.2 Print your home directory using echo.

```
[ese-wangyy@login02 ~]$ echo $HOME
/work/ese-wangyy
```

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

```
[ese-wangyy@login02 ~]$ cd data_demo/molecules
[ese-wangyy@login02 molecules]$ touch test.pdb
[ese-wangyy@login02 molecules]$ ll
total 3
-rwxr-xr-x 1 ese-wangyy ese-ouycc 1158 Nov 24 19:24 cubane.pdb
-rwxr-xr-x 1 ese-wangyy ese-ouycc  622 Nov 24 19:24 ethane.pdb
-rwxr-xr-x 1 ese-wangyy ese-ouycc  422 Nov 24 19:24 methane.pdb
-rwxr-xr-x 1 ese-wangyy ese-ouycc 1828 Nov 24 19:24 octane.pdb
-rwxr-xr-x 1 ese-wangyy ese-ouycc 1226 Nov 24 19:24 pentane.pdb
-rwxr-xr-x 1 ese-wangyy ese-ouycc  825 Nov 24 19:24 propane.pdb
-rw-r--r-- 1 ese-wangyy ese-ouycc    0 Dec  3 19:15 test.pdb
```

1.4 Find how many files in data_demo/data/elements/ using find.

```
[ese-wangyy@login02 elements]$ find ./ -type f | wc -l
103
```

参考资料：

<https://www.cnblogs.com/kingsonfu/p/11683494.html>

1.5 Compare data_demo/data/pdb/ethane.pdb and data_demo/data/pdb/ethanol.pdb with diff.

```
[ese-wangyy@login02 ~]$ 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
```

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

```
[ese-wangyy@login02 ~]$ grep "But she" data_demo/writing/data/LittleWomen.txt | wc -l
15
```

1.7 Check the total file size of the data_demo/data/ folder using du.

```
[ese-wangyy@login02 ~]$ du -h data_demo/data/  
408K    data_demo/data/pdb  
52K     data_demo/data/elements  
1.0K    data_demo/data/animal-counts  
719K    data_demo/data/
```

1.8 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.

```
[ese-wangyy@login02 ~]$ cp -r data_demo/writing/ data_demo/writing_new/  
[ese-wangyy@login02 ~]$ cd data_demo  
[ese-wangyy@login02 data_demo]$ ll  
total 133  
drwxr-xr-x 2 ese-wangyy ese-ouycc 4096 Nov 24 19:24 creatures  
drwxr-xr-x 5 ese-wangyy ese-ouycc 4096 Nov 24 19:24 data  
-rw-r--r-- 1 ese-wangyy ese-ouycc 587 Dec 3 16:41 log1  
drwxr-xr-x 2 ese-wangyy ese-ouycc 4096 Dec 3 19:15 molecules  
drwxr-xr-x 3 ese-wangyy ese-ouycc 4096 Nov 24 19:24 north-pacific-gyre  
-rw-r-xr-x 1 ese-wangyy ese-ouycc 69 Nov 24 19:24 notes  
-rw-r-xr-x 1 ese-wangyy ese-ouycc 32 Nov 24 19:24 pizza.cfg  
-rw-r-xr-x 1 ese-wangyy ese-ouycc 21583 Nov 24 19:24 solar.pdf  
drwxr-xr-x 2 ese-wangyy ese-ouycc 4096 Nov 24 20:35 thesis  
drwxr-xr-x 5 ese-wangyy ese-ouycc 4096 Nov 24 19:24 writing  
drwxr-xr-x 5 ese-wangyy ese-ouycc 4096 Dec 3 20:03 writing_new
```

```
[ese-wangyy@login02 data_demo]$ ll  
total 133  
drwxr-xr-x 2 ese-wangyy ese-ouycc 4096 Nov 24 19:24 creatures  
drwxr-xr-x 5 ese-wangyy ese-ouycc 4096 Nov 24 19:24 data  
-rw-r--r-- 1 ese-wangyy ese-ouycc 587 Dec 3 16:41 log1  
drwxr-xr-x 2 ese-wangyy ese-ouycc 4096 Dec 3 19:15 molecules  
drwxr-xr-x 3 ese-wangyy ese-ouycc 4096 Nov 24 19:24 north-pacific-gyre  
-rw-r-xr-x 1 ese-wangyy ese-ouycc 69 Nov 24 19:24 notes  
-rw-r-xr-x 1 ese-wangyy ese-ouycc 32 Nov 24 19:24 pizza.cfg  
-rw-r-xr-x 1 ese-wangyy ese-ouycc 21583 Nov 24 19:24 solar.pdf  
drwxr-xr-x 2 ese-wangyy ese-ouycc 4096 Nov 24 20:35 thesis  
drwxr-xr-x 5 ese-wangyy ese-ouycc 4096 Nov 24 19:24 writing  
drwxr-xr-x 5 ese-wangyy ese-ouycc 4096 Dec 3 20:11 writing_new  
[ese-wangyy@login02 data_demo]$ zip -q -r writing_new.zip *  
[ese-wangyy@login02 data_demo]$ ll  
total 133  
drwxr-xr-x 2 ese-wangyy ese-ouycc 4096 Nov 24 19:24 creatures  
drwxr-xr-x 5 ese-wangyy ese-ouycc 4096 Nov 24 19:24 data  
-rw-r--r-- 1 ese-wangyy ese-ouycc 587 Dec 3 16:41 log1  
drwxr-xr-x 2 ese-wangyy ese-ouycc 4096 Dec 3 19:15 molecules  
drwxr-xr-x 3 ese-wangyy ese-ouycc 4096 Nov 24 19:24 north-pacific-gyre  
-rw-r-xr-x 1 ese-wangyy ese-ouycc 69 Nov 24 19:24 notes  
-rw-r-xr-x 1 ese-wangyy ese-ouycc 32 Nov 24 19:24 pizza.cfg  
-rw-r-xr-x 1 ese-wangyy ese-ouycc 21583 Nov 24 19:24 solar.pdf  
drwxr-xr-x 2 ese-wangyy ese-ouycc 4096 Nov 24 20:35 thesis  
drwxr-xr-x 5 ese-wangyy ese-ouycc 4096 Nov 24 19:24 writing  
drwxr-xr-x 5 ese-wangyy ese-ouycc 4096 Dec 3 20:11 writing_new  
-rw-r--r-- 1 ese-wangyy ese-ouycc 998359 Dec 3 20:12 writing_new.zip
```

```
[ese-wangyy@login02 data_demo]$ unzip writing_new.zip  
Archive: writing_new.zip  
replace creatures/basilisk.dat? [y]es, [n]o, [A]ll, [N]one, [r]ename: A  
  inflating: creatures/basilisk.dat  
  inflating: creatures/minotaur.dat
```

1.9 Change the file permissions flags on writing_new to drwxr-x--- using chmod.

```
[ese-wangyy@login02 data_demo]$ chmod 750 writing_new/  
[ese-wangyy@login02 data_demo]$ ll  
total 1157  
drwxr-xr-x 2 ese-wangyy ese-ouycc 4096 Dec 3 20:18 creatures  
drwxr-xr-x 5 ese-wangyy ese-ouycc 4096 Dec 3 20:18 data  
-rw-r--r-- 1 ese-wangyy ese-ouycc 587 Dec 3 16:41 log1  
drwxr-xr-x 2 ese-wangyy ese-ouycc 4096 Dec 3 20:18 molecules  
drwxr-xr-x 3 ese-wangyy ese-ouycc 4096 Nov 24 19:24 north-pacific-gyre  
-rw-r-xr-x 1 ese-wangyy ese-ouycc 69 Nov 24 19:24 notes  
-rw-r-xr-x 1 ese-wangyy ese-ouycc 32 Nov 24 19:24 pizza.cfg  
-rw-r-xr-x 1 ese-wangyy ese-ouycc 21583 Nov 24 19:24 solar.pdf  
drwxr-xr-x 2 ese-wangyy ese-ouycc 4096 Nov 24 20:35 thesis  
drwxr-xr-x 5 ese-wangyy ese-ouycc 4096 Dec 3 20:18 writing  
drwxr-x--- 5 ese-wangyy ese-ouycc 4096 Dec 3 20:11 writing_new  
-rw-r--r-- 1 ese-wangyy ese-ouycc 998359 Dec 3 20:12 writing_new.zip
```

1.10 Print the last 10 commands you made using history.

```
[ese-wangyy@login02 ~]$ history 10
325  ll
326  chmod drwxr-x---writing_new
327  chmod drwxr-x writing_new
328  chmod --help
329  chmod drwxr-xr writing_new
330  chmod drwxr-x---writing_new
331  ll
332  cd ~
333  history
334  history 10
```


2. BASH for Loop

The general syntax of a BASH loop goes like:

```
for thing in list_of_things
do
    operation_using $thing
done
```

(龚国庆向我解释了此题) Write a shell script to print file size (in bytes) of each *.pdb file in data_demo/data/pdb/, line by line.

先创建一个 loop.sh，并进入编辑，使用 for 循环读取 data_demo/data/pdb/*.pdb，再用 du -b 读取文件大小。

```
[ese-wangyy@login02 ~]$ vi loop.sh
for i in data_demo/data/pdb/*.pdb
do
    du -b $i
done
```

最后运行 loop.sh 得到结果：

```
[ese-wangyy@login02 ~]$ chmod 750 loop.sh
[ese-wangyy@login02 ~]$ ./loop.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
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
```