

## 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/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

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

[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
```

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