

1 Linux Commands

```
[ese-zhanglc@login02 ~]$ cd ~  
[ese-zhanglc@login02 ~]$ ls  
data_demo  exam  mpi_demo
```

1.1

```
[ese-zhanglc@login02 ~]$ ln -s data_demo data_demo_link  
[ese-zhanglc@login02 ~]$ ls -l  
total 2  
drwxr-xr-x 7 ese-zhanglc ese-ouycc 4096 Dec  3 16:49 data_demo  
lrwxrwxrwx 1 ese-zhanglc ese-ouycc    9 Dec  6 23:53 data_demo_link -> data_demo  
drwxr-xr-x 2 ese-zhanglc ese-ouycc 4096 Nov  2 18:47 exam  
drwxr-xr-x 2 ese-zhanglc ese-ouycc 4096 Dec  3 18:00 mpi_demo
```

1.2

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

1.3

```
[ese-zhanglc@login02 ~]$ cd data_demo/molecules/  
[ese-zhanglc@login02 molecules]$ touch test.pdb  
[ese-zhanglc@login02 molecules]$ ls -l  
total 3  
-rwxr-xr-x 1 ese-zhanglc ese-ouycc 1158 Dec  1 19:08 cubane.pdb  
-rwxr-xr-x 1 ese-zhanglc ese-ouycc  622 Dec  1 19:08 ethane.pdb  
-rwxr-xr-x 1 ese-zhanglc ese-ouycc  422 Dec  1 19:08 methane.pdb  
-rwxr-xr-x 1 ese-zhanglc ese-ouycc 1828 Dec  1 19:08 octane.pdb  
-rwxr-xr-x 1 ese-zhanglc ese-ouycc 1226 Dec  1 19:08 pentane.pdb  
-rwxr-xr-x 1 ese-zhanglc ese-ouycc  825 Dec  1 19:08 propane.pdb  
-rw-r--r-- 1 ese-zhanglc ese-ouycc    0 Dec  7 00:07 test.pdb
```

1.4

```
[ese-zhanglc@login02 molecules]$ cd ..  
[ese-zhanglc@login02 data_demo]$ cd data/elements/  
[ese-zhanglc@login02 elements]$ find -type f | wc -l  
103
```

```
[ese-zhanglc@login02 ~]$ ls data_demo/data/elements | wc -l  
103
```

1.5

```
[ese-zhanglc@login02 ~]$ cd data_demo/data/pdb
[ese-zhanglc@login02 pdb]$ ls
aldrin.pdb      citronellal.pdb  ethanol.pdb      lsd.pdb          mustard.pdb      print.sh.save    testosterone.pdb  vitamin-a.pdb
ammonia.pdb     codeine.pdb      ethylcyclohexane.pdb  maltose.pdb      nerol.pdb        propane.pdb      thiamine.pdb
ascorbic-acid.pdb  cubane.pdb       glycol.pdb        menthol.pdb      norethndrone.pdb  pyridoxal.pdb   tyrian.pdb
benzaldehyde.pdb  cyclobutane.pdb  heme.pdb          methanol.pdb     octane.pdb        quinine.pdb     tuber.in.pdb
camphene.pdb     cyclohexanol.pdb  lactic-acid.pdb   methanol.pdb     pentane.pdb       strychnine.pdb  tyrian-purple.pdb
cholesterol.pdb   cyclopropane.pdb  lactose.pdb       mint.pdb         piperine.pdb     styrene.pdb     vanillin.pdb
cinnamaldehyde.pdb ethane.pdb        lanoxin.pdb       morphine.pdb     print.sh          sucrose.pdb     vinyl-chloride.pdb

[ese-zhanglc@login02 pdb]$ diff ethane.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-zhanglc@login02 data]$ cd ..
[ese-zhanglc@login02 data_demo]$ cd writing/data/
[ese-zhanglc@login02 data]$ grep -o "But she" LittleWomen.txt | wc -l
15
```

1.7

```
[ese-zhanglc@login02 pdb]$ cd ..
[ese-zhanglc@login02 data]$ du -sh
720K .
```

1.8

```
[ese-zhanglc@login02 writing]$ cd ..
[ese-zhanglc@login02 data_demo]$ ls
creatures data log1 log2 molecules north-pacific-gyre notes pizza.cfg solar.pdf temp writing
[ese-zhanglc@login02 data_demo]$ mkdir writing_new
[ese-zhanglc@login02 data_demo]$ ls
creatures data log1 log2 molecules north-pacific-gyre notes pizza.cfg solar.pdf temp writing writing_new
[ese-zhanglc@login02 data_demo]$ cp -r writing writing_new
[ese-zhanglc@login02 data_demo]$ cd writing_new
[ese-zhanglc@login02 writing_new]$ ls
writing

[ese-zhanglc@login02 data_demo]$ zip -r writing_new.zip writing_new
adding: writing_new/ (stored 0%)
adding: writing_new/writing/ (stored 0%)
adding: writing_new/writing/haiku.txt (deflated 29%)
adding: writing_new/writing/tools/ (stored 0%)
adding: writing_new/writing/tools/stats (stored 0%)
adding: writing_new/writing/tools/old/ (stored 0%)
adding: writing_new/writing/tools/old/oldtool (stored 0%)
adding: writing_new/writing/tools/format (deflated 13%)
adding: writing_new/writing/data/ (stored 0%)
adding: writing_new/writing/data/one.txt (deflated 53%)
adding: writing_new/writing/data/LittleWomen.txt (deflated 61%)
adding: writing_new/writing/data/two.txt (deflated 59%)
adding: writing_new/writing/thesis/ (stored 0%)
adding: writing_new/writing/thesis/empty-draft.md (stored 0%)
[ese-zhanglc@login02 data_demo]$ ls
creatures data log1 log2 molecules north-pacific-gyre notes pizza.cfg solar.pdf temp writing writing_new writing_new.zip
[ese-zhanglc@login02 data_demo]$ unzip writing_new.zip
Archive:  writing_new.zip
replace writing_new/writing/haiku.txt? [y]es, [n]o, [A]ll, [N]one, [r]ename: A
  inflating: writing_new/writing/haiku.txt
  extracting: writing_new/writing/tools/stats
  extracting: writing_new/writing/tools/old/oldtool
  inflating: writing_new/writing/tools/format
  inflating: writing_new/writing/data/one.txt
  inflating: writing_new/writing/data/LittleWomen.txt
  inflating: writing_new/writing/data/two.txt
  extracting: writing_new/writing/thesis/empty-draft.md
[ese-zhanglc@login02 data_demo]$
```

1.9

```
[ese-zhanglc@login02 data_demo]$ chmod 755 writing_new
[ese-zhanglc@login02 data_demo]$ ls
creatures data log1 log2 molecules north-pacific-gyre notes pizza.cfg solar.pdf temp writing writing_new writing_new.zip
```

1.10

```
[ese-zhanglc@login02 data_demo]$ history 10
173 zip -q -r writing_new.zip
174 cd ..
175 zip -q -r writing_new.zip
176 zip -r writing_new.zip
177 zip -r writing_new.zip writing_new
178 ls
179 unzip writing_new.zip
180 chmod 755 writing_new
181 ls
182 history 10
```

2 BASH for Loop

```
[ese-zhanglc@login03 pdb]$ ls
aldrin.pdb      cubane.pdb      lactic-acid.pdb  mint.pdb        print.sh.save    tnt.pdb
ammonia.pdb     cyclobutane.pdb lactose.pdb       morphine.pdb     propane.pdb      tuberin.pdb
ascorbic-acid.pdb cyclohexanol.pdb lanoxin.pdb       mustard.pdb      pyridoxal.pdb    tyrian-purple.pdb
benzaldehyde.pdb cyclopropane.pdb loop-filefolder.sh nerol.pdb        quinine.pdb      vanillin.pdb
camphene.pdb    ethane.pdb       lsd.pdb           norethindrone.pdb strychnine.pdb   vinyl-chloride.pdb
cholesterol.pdb ethanol.pdb        maltose.pdb       octane.pdb       styrene.pdb      vitamin-a.pdb
cinnamaldehyde.pdb ethylcyclohexane.pdb menthol.pdb      pentane.pdb      sucrose.pdb      testosterone.pdb
citronellal.pdb glycol.pdb        methane.pdb       piperine.pdb     thiamine.pdb
codeine.pdb     heme.pdb         methanol.pdb
[ese-zhanglc@login03 pdb]$ bash loop-filefolder.sh
1 aldrin.pdb
1 ammonia.pdb
1 ascorbic-acid.pdb
1 benzaldehyde.pdb
1 camphene.pdb
128 cholesterol.pdb
1 cinnamaldehyde.pdb
1 citronellal.pdb
1 codeine.pdb
1 cubane.pdb
1 cyclobutane.pdb
1 cyclohexanol.pdb
1 cyclopropane.pdb
1 ethane.pdb
1 ethanol.pdb
1 ethylcyclohexane.pdb
1 glycol.pdb
128 heme.pdb
```

```
1 lactic-acid.pdb
1 lactose.pdb
128 lanoxin.pdb
1 lsd.pdb
1 maltose.pdb
1 menthol.pdb
1 methane.pdb
1 methanol.pdb
1 mint.pdb
1 morphine.pdb
1 mustard.pdb
1 nerol.pdb
1 norethindrone.pdb
1 octane.pdb
1 pentane.pdb
1 piperine.pdb
1 propane.pdb
1 pyridoxal.pdb
1 quinine.pdb
1 strychnine.pdb
1 styrene.pdb
1 sucrose.pdb
1 testosterone.pdb
1 thiamine.pdb
1 tnt.pdb
1 tuberin.pdb
1 tyrian-purple.pdb
1 vanillin.pdb
1 vinyl-chloride.pdb
1 vitamin-a.pdb
```