1.1

1.2

```
[ese-zhaijw@login01 ~]$ echo "ls $HOME"
ls /work/ese-zhaijw
```

1.3

```
[ese-zhaijw@login01 ~]$ cd data_demo
[ese-zhaijw@login01 data_demo]$ cd molecules
\[ese-zhaijw@login01 molecules]$ touch test.pdb
[ese-zhaijw@login01 molecules]$ ls
cubane.pdb ethane.pdb methane.pdb octane.pdb pentane.pdb propane.pdb test.pdb
```

1 /

```
[ese-zhaijw@login01 ~]$ find data_demo/data/elements/
data_demo/data/elements/
data demo/data/elements/Md.xml
data_demo/data/elements/In.xml
data_demo/data/elements/Bk.xml
data demo/data/elements/Eu.xml
data_demo/data/elements/Cd.xml
data_demo/data/elements/Pb.xml
data demo/data/elements/Th.xml
data_demo/data/elements/Pr.xml
data_demo/data/elements/Ac.xml
data demo/data/elements/As.xml
data_demo/data/elements/Ca.xml
data_demo/data/elements/Li.xml
data_demo/data/elements/H.xml
data_demo/data/elements/Te.xml
data demo/data/elements/Po.xml
data_demo/data/elements/Fr.xml
```

```
[ese-zhaijw@login03 ~]$ find data_demo/data/elements/ -name "*.*" | wc -l
103
```

1.5

```
[ese-zhaijw@login01 pdb]$ diff ethane.pdb ethanol.pdb
1,11c1,12
< COMPND ETHANE
< AUTHOR DAVE WOODCOCK 95 12 18
  ATOM
                                                            -0.752
0.752
-1.158
                                                                            0.001
                                                                                         -0.141
                                                                                                       1.00
                                                                                                                 0.00
                    123456789
                                                                                          0.141
0.070
                                                                                                       1.00
1.00
1.00
                                                                                                                 0.00
0.00
0.00
  ATOM
                                                                           -0.001
  MOTA
MOTA
MOTA
                                                                           0.991
                         HHHHH
                                                            -1.240
                                                                          -0.737
-0.249
                                                                                          0.496
                                                            -0.924
                                                                                         -1.188
                                                                                                                 0.00
                                                                                                       1.00
  MOTA
                                                             1.158
                                                                           -0.991
                                                                                          -0.070
                                                                                                       1.00
  MOTA
                                                             0.924
                                                                           0.249
                                                                                         1.188
-0.496
                                                                                                       1.00
                                                                                                                 0.00
  ATOM
TER
  COMPND
AUTHOR
                        ETHANOL
                       DAVE WOODCOCK 96 01 03
                                                           -0.426
-0.599
-0.750
-1.022
  ATOM
                         C
0
                    1
2
3
4
5
                                                                          -0.115
                                                                                         -0.147
                                                                                                                 0.00
  ATOM
ATOM
ATOM
ATOM
                                                                                                                 0.00
0.00
0.00
                                                                          1.244
-0.738
-0.351
                                                                                         -0.481
-0.981
                                                                                                       1.00
                                                                                                       1.00
                         HHUUHHH
                                                                                          0.735
0.689
                                                             -1.642
                                                                            1.434
                                                                                                       1.00
  ATOM
ATOM
ATOM
                                                             1.047
1.370
1.642
                                                                          -0.383
0.240
-0.147
                                                                                          0.147
0.981
-0.735
                                                                                                                 0.00
0.00
0.00
                                                                                                       1.00
                    6
7
8
9
                                                                                                       1.00
  ATOM
TER
                   10
```

```
[ese-zhaijw@login03 data]$ grep "But she" LittleWomen.txt
"Oh, bless you, no! But she let old Belsham rest, and when I ran back
small quaver in her voice, "I came to thank you, sir, for..." But she
than she went. But she begged so hard, and Sallie had promised to take
But she does not hunt as our darling did,
But she only spits at the dogs our pet
But she is not fair to see,
queer thing for her to do, she doesn't act a bit like herself. But she
aspirant for fame, with philosophic composure. But she made a wry face
her. But she can pet and comfort him after I'm gone, and so cure him
to see signs of hope in the faint color on Beth's cheeks. But she
But she did not get it, for though he joined her and answered all her
sketchbook. But she tucked it under her arm with a sharp...
Amy did any of these fond and foolish things. But she certainly did
But she did show something better than brilliancy or skill, for she
grasshopper. But she would have consented if he had proposed to sing a
```

```
[ese-zhaijw@login03 ~]$ grep "But she" data demo/writing/data/LittleWomen.txt -o | wc -l
```

1.7

```
[ese-zhaijw@login03 data]$ du -c
        ./pdb
537
52
        ./elements
        ./animal-counts
849
849
        total
```

1.8

```
[ese-zhaijw@login03 data_demo]$ cp -r writing writing_new
[ese-zhaijw@login03 data_demo]$ ls
creatures data molecules north-pacific-gyre notes pizza.cfg solar.pdf test writing_new
[ese-zhaijw@login03 data_demo]$ zip -r writing_new.zip writing_new
adding: writing_new/(stored 0%)
adding: writing_new/tools/ (stored 0%)
adding: writing_new/tools/ (stored 0%)
adding: writing_new/tools/old/ (stored 0%)
adding: writing_new/tools/old/ (stored 0%)
adding: writing_new/tools/old/oldtool (stored 0%)
adding: writing_new/tools/old/oldtool (stored 0%)
adding: writing_new/data/format (deflated 13%)
adding: writing_new/data/ (stored 0%)
adding: writing_new/data/titleWomen.txt (deflated 61%)
adding: writing_new/data/two.txt (deflated 59%)
adding: writing_new/data/two.txt (deflated 59%)
adding: writing_new/thesis/empty-draft.md (stored 0%)
[ese-zhaijw@login03 data_demo]$ unzip writing_new.zip

Archive: writing_new.zip
```

19

```
[ese-zhaijw@login03 data_demo]$ chmod 750 writing_new
[ese-zhaijw@login03 data_demo]$ ls -l
  total 645
drwxr-xr-x 2 ese-zhaijw ese-ouycc
drwxr-xr-x 5 ese-zhaijw ese-ouycc
drwxr-xr-x 2 ese-zhaijw ese-ouycc
drwxr-xr-x 3 ese-zhaijw ese-ouycc
                                                                                                                                                                                                                                                4096 Nov 24 19:25 creatures
4096 Nov 24 19:25 data
                                                                                                                                                                                                                                                 4096 Dec 3 17:16 molecules
4096 Nov 24 19:25 north-pacific-gyre
drwxr-xr-x 3 ese-zhaljw ese-ouycc
-rwxr-xr-x 1 ese-zhaljw ese-ouycc
-rwxr-xr-x 1 ese-zhaljw ese-ouycc
-rwxr-xr-x 1 ese-zhaljw ese-ouycc
drwxr-xr-x 2 ese-zhaljw ese-ouycc
drwxr-xr-x 5 ese-zhaljw ese-ouycc
drwxr-xr-x 5 ese-zhaljw ese-ouycc
drwxr-xr-x 6 ese-zhaljw ese-ouycc
drwxr-xr-x 7 ese-zhaljw ese-ouycc
drwxr-xr-x 8 ese-zhaljw ese-ouycc
drwxr-xr-x 9 ese-zhaljw ese-ouycc
drwxr-xr-x 1 ese-zhaljw ese-ouycc
drwxr-xr-x 2 ese-zhaljw ese-ouycc
drwxr-xr-x 5 ese-zhaljw ese-ouycc
```

```
[ese-zhaijw@login03 ~]$ history 10
  341
        ls -
       chmod 710 writing_new
chmod 710 writing_new.sh
  342
  343
  344
       cd ..
       chmod 710 writing_new
  345
  346
        ls -l
       chmod 750 writing new
  347
  348
       ls -l
       cd ..
  349
  350
       history 10
```

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

```
for fname in *.pdb
do
du -b $fname
done
```