

## 1.1

```
[ese-zhaijw@login03 ~]$ ls
data_demo err.log exam job2.log job.log job.sh mpi_demo result.log result.log2 t1.py t2.py
[ese-zhaijw@login03 ~]$ ln -s data_demo data_demo_link
[ese-zhaijw@login03 ~]$ ls
data_demo data_demo_link err.log exam job2.log job.log job.sh mpi_demo result.log result.log2 t1.py t2.py
```

## 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
```

## 1.4

```
[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 "*.xml" | 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        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-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
15
```

1.7

```
[ese-zhaijw@login03 data]$ du -c
537    ./pdb
52     ./elements
1      ./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  writing_new
[ese-zhaijw@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-zhaijw@login03 data_demo]$ unzip writing_new.zip
Archive:  writing_new.zip
```

1.9

```
[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 4096 Nov 24 19:25 creatures
drwxr-xr-x 5 ese-zhaijw ese-ouycc 4096 Nov 24 19:25 data
drwxr-xr-x 2 ese-zhaijw ese-ouycc 4096 Dec 3 17:16 molecules
drwxr-xr-x 3 ese-zhaijw ese-ouycc 4096 Nov 24 19:25 north-pacific-gyre
-rwxr-xr-x 1 ese-zhaijw ese-ouycc 76 Dec 1 16:28 notes
-rwxr-xr-x 1 ese-zhaijw ese-ouycc 32 Dec 1 16:28 pizza.cfg
-rwxr-xr-x 1 ese-zhaijw ese-ouycc 21583 Dec 1 16:28 solar.pdf
drwxr-xr-x 2 ese-zhaijw ese-ouycc 4096 Nov 24 20:22 test
drwxr-xr-x 5 ese-zhaijw ese-ouycc 4096 Nov 24 19:25 writing
drwxr-xr-x 5 ese-zhaijw ese-ouycc 4096 Dec 4 10:31 writing_new
-rw-r--r-- 1 ese-zhaijw ese-ouycc 422584 Dec 4 10:34 writing_new.zip
```

1.10

```
[ese-zhaijw@login03 ~]$ history 10
341  ls -l
342  chmod 710 writing_new
343  chmod 710 writing_new.sh
344  cd ..
345  chmod 710 writing_new
346  ls -l
347  chmod 750 writing_new
348  ls -l
349  cd ..
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
1444  ascorbic-acid.pdb
1030  benzaldehyde.pdb
1830  camphene.pdb
5049  cholesterol.pdb
1090  cinnamaldehyde.pdb
1694  citronellal.pdb
2452  codeine.pdb
1158  cubane.pdb
895   cyclobutane.pdb
1384  cyclohexanol.pdb
695   cyclopropane.pdb
622   ethane.pdb
690   ethanol.pdb
2396  ethylcyclohexane.pdb
765   glycol.pdb
4209  heme.pdb
1064  lactic-acid.pdb
2562  lactose.pdb
11193 lanoxin.pdb
3395  lsd.pdb
```

GNU nano 2.3.1

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