# [ese-wurx@login03 ~]\$ ln -s data\_demo data\_demo\_link

```
[ese-wurx@login03 ~]$ ll
total 2
drwxr-xr-x 7 ese-wurx ese-ouycc 4096 Dec 1 20:22 data_demo
lrwxrwxrwx 1 ese-wurx ese-ouycc 9 Dec 7 19:06 data_demo_link -> data_demo
drwxr-xr-x 2 ese-wurx ese-ouycc 4096 Nov 2 18:47 exam
drwxr-xr-x 2 ese-wurx ese-ouycc 4096 Dec 3 17:59 mpi_demo
```

## **1.2**

```
[ese-wurx@login03 data_demo]$ echo $HOME
/work/ese-wurx
```

## **1.3**

```
[ese-wurx@login03 ~]$ cd data_demo/molecules/
[ese-wurx@login03 molecules]$ pwd
/work/ese-wurx/data demo/molecules
```

```
[ese-wurx@login03 molecules]$ touch test.pdb
[ese-wurx@login03 molecules]$ ll
total 3
-rwxr-xr-x 1 ese-wurx ese-ouycc 1158 Dec 1 19:41 cubane.pdb
-rwxr-xr-x 1 ese-wurx ese-ouycc 622 Dec 1 19:41 ethane.pdb
-rwxr-xr-x 1 ese-wurx ese-ouycc 422 Dec 1 19:41 methane.pdb
-rwxr-xr-x 1 ese-wurx ese-ouycc 1828 Dec 1 19:41 octane.pdb
-rwxr-xr-x 1 ese-wurx ese-ouycc 1226 Dec 1 19:41 pentane.pdb
-rwxr-xr-x 1 ese-wurx ese-ouycc 825 Dec 1 19:41 propane.pdb
-rw-r--r-- 1 ese-wurx ese-ouycc 0 Dec 7 19:15 test.pdb
```

#### 1.4

```
[ese-wurx@login03 ~]$ cd data_demo/data/elements/
[ese-wurx@login03 elements]$ pwd
/work/ese-wurx/data_demo/data/elements
[ese-wurx@login03 elements]$ find . -type f -print | wc -l
103
```

```
[ese-wurx@login03 ~]$ cd data_demo/data/pdb/
[ese-wurx@login03 pdb]$ diff ethane.pdb ethanol.pdb
1,11c1,12
< COMPND
              ETHANE
              DAVE WOODCOCK 95 12 18
< AUTHOR
< ATOM
            1 C
                                  -0.752
                                          0.001
                                                 -0.141 1.00
                                                                0.00
                                                         1.00
1.00
< ATOM
            2
                                  0.752
                                          -0.001
                                                  0.141
                                                                0.00
            3
              Н
< ATOM
                           1
                                  -1.158
                                          0.991
                                                   0.070
                                                                0.00
                                  -1.240
                                                  0.496
< ATOM
                                          -0.737
                                                         1.00
                                                                0.00
            5
              Н
                                  -0.924
                                          -0.249
< ATOM
                                                 -1.188
                                                         1.00
                                                                0.00
            6
< ATOM
              Н
                                  1.158
                                          -0.991
                                                 -0.070 1.00
                                                                0.00
                                                  1.188 1.00
                           1
                                   0.924
                                          0.249
< ATOM
              Н
                                                               0.00
< ATOM
            8
              Н
                           1
                                   1.240
                                           0.737
                                                  -0.496 1.00
                                                               0.00
< TER
            9
                           1
> COMPND
              ETHANOL
> AUTHOR
              DAVE WOODCOCK 96 01 03
> ATOM
                                  -0.426
                                         -0.115 -0.147 1.00
                                                                0.00
                                          1.244
            2 0
> ATOM
                                  -0.599
                                                 -0.481
                                                         1.00
                                                                0.00
            3
                                                         1.00
> ATOM
              Н
                                  -0.750
                                         -0.738
                                                  -0.981
                                                                0.00
> ATOM
            4
              Н
                           1
                                  -1.022
                                          -0.351
                                                  0.735
                                                          1.00
                                                                0.00
            5
                           1
> ATOM
              Н
                                  -1.642
                                          1.434
                                                  -0.689
                                                          1.00
                                                                0.00
            6
> ATOM
              C
                                  1.047
                                          -0.383
                                                  0.147
                                                         1.00
                                                                0.00
                           1
                                                   0.981 1.00
 MOTA
              Н
                           1
                                   1.370
                                          0.240
                                                                0.00
            8
 MOTA
              Н
                                   1.642
                                         -0.147
                                                  -0.735 1.00
                                                               0.00
            9
                                                  0.405 1.00
                           1
                                         -1.434
> ATOM
              Н
                                   1.180
                                                               0.00
> TER
           10
                           1
```

#### 1.6

```
[ese-wurx@login03 ~]$ cd data_demo/writing/data/
[ese-wurx@login03 data]$ grep -c 'But she' LittleWomen.txt
15
```

#### 1.7

```
[ese-wurx@login03 data]$ du -sh
1.3M .
[ese-wurx@login03 data]$ du -sh * | sort -n
1.2M LittleWomen.txt
128K two.txt
512 one.txt
```

#### Copy:

```
[ese-wurx@login03 ~]$ cp -r data demo/writing/ data demo/writing new/
[ese-wurx@login03 ~]$ cd data_demo
[ese-wurx@login03 data_demo]$ ll
total 135
drwxr-xr-x 2 ese-wurx ese-ouycc 4096 Dec
                                          1 19:41 creatures
drwxr-xr-x 5 ese-wurx ese-ouycc 4096 Dec 1 19:41 data
                                 0 Dec 1 20:22 err.log
-rw-r--r-- 1 ese-wurx ese-ouycc
                               1822 Dec
                                         1 20:22 job.log
-rw-r--r-- 1 ese-wurx ese-ouycc
                                380 Dec
-rw-r--r-- 1 ese-wurx ese-ouycc
                                         1 19:55 job.sh
drwxr-xr-x 2 ese-wurx ese-ouycc 4096 Dec 7 19:15 molecules
drwxr-xr-x 3 ese-wurx ese-ouycc 4096 Dec 1 19:41 north-pacific-gyre
                                 76 Dec 1 19:41 notes
-rwxr-xr-x 1 ese-wurx ese-ouycc
                                  32 Dec 1 19:41 pizza.cfg
-rwxr-xr-x 1 ese-wurx ese-ouycc
-rw-r--r-- 1 ese-wurx ese-ouycc 45 Dec
                                          1 20:22 result.log
-rwxr-xr-x 1 ese-wurx ese-ouycc 21583 Dec
                                          1 19:41 solar.pdf
                                          1 19:52 t1.py
                                 222 Dec
-rw-r--r-- 1 ese-wurx ese-ouycc
                                  20 Dec
                                          1 19:41 temp
-rw-r--r-- 1 ese-wurx ese-ouycc
drwxr-xr-x 5 ese-wurx ese-ouycc 4096 Dec 1 19:41 writing
drwxr-xr-x 5 ese-wurx ese-ouycc 4096 Dec 7 20:17 writing_new
```

## Zip:

```
[ese-wurx@login03 data demo]$ zip -r writing new.zip *
```

```
[ese-wurx@login03 data demo]$ ll
total 135
drwxr-xr-x 2 ese-wurx ese-ouycc
                                  4096 Dec 1 19:41 creatures
                                  4096 Dec 1 19:41 data
drwxr-xr-x 5 ese-wurx ese-ouycc
-rw-r--r-- 1 ese-wurx ese-ouycc
                                    0 Dec 1 20:22 err.log
                                  -rw-r--r-- 1 ese-wurx ese-ouycc
-rw-r--r-- 1 ese-wurx ese-ouycc
drwxr-xr-x 2 ese-wurx ese-ouycc
                                 4096 Dec 7 19:15 molecules
                                 4096 Dec 1 19:41 north-pacific-gyre
drwxr-xr-x 3 ese-wurx ese-ouycc
                                   76 Dec 1 19:41 notes
-rwxr-xr-x 1 ese-wurx ese-ouycc
                                    32 Dec 1 19:41 pizza.cfg
-rwxr-xr-x 1 ese-wurx ese-ouycc
                                   45 Dec 1 20:22 result.log
-rw-r--r-- 1 ese-wurx ese-ouycc
                                 21583 Dec 1 19:41 solar.pdf
-rwxr-xr-x 1 ese-wurx ese-ouycc
-rw-r--r-- 1 ese-wurx ese-ouycc
                                   222 Dec 1 19:52 t1.py
-rw-r--r-- 1 ese-wurx ese-ouycc
                                   20 Dec 1 19:41 temp
                                  4096 Dec 1 19:41 writing
drwxr-xr-x 5 ese-wurx ese-ouycc
                                  4096 Dec 7 20:17 writing_new
drwxr-xr-x 5 ese-wurx ese-ouycc
-rw-r--r-- 1 ese-wurx ese-ouycc 1000201 Dec 7 20:24 writing new.zip
```

## Unzip:

```
[ese-wurx@login03 data_demo]$ unzip -n writing_new.zip
Archive: writing_new.zip
```

```
[ese-wurx@login03 data_demo]$ chmod 750 writing_new
```

```
drwxr-x--- 5 ese-wurx ese-ouycc 4096 Dec 7 20:17 writing_new
```

## 1.10

```
[ese-wurx@login03 data_demo]$ history 10
   144  unzip -n writing_new.zip
   145  ll
   146  chmod drwxr-x--- writing_new
   147  chmod d rwxr-x--- writing_new
   148  ll
   149  chmod 750 writing_new
   150  ll
   151  history -10
   152  history -w -10
   153  history 10
```

#### 2

## #I got inspired by Zhou Yunqiu

```
[ese-wurx@login03 ~]$ cd data_demo/data/pdb/
[ese-wurx@login03 pdb]$ nano loop.sh
```

## loop.sh:

```
for pdb in *.pdb
do
du -a -h $pdb
done
```

```
[ese-wurx@login03 pdb]$ chmod 750 loop.sh
[ese-wurx@login03 pdb]$ ./loop.sh
```

#### **Result:**

```
aldrin.pdb
512
         ammonia.pdb
512
512
         ascorbic-acid.pdb
         benzaldehyde.pdb
512
         camphene.pdb
128K
         cholesterol.pdb
512
         cinnamaldehyde.pdb
512
         citronellal.pdb
512
512
         codeine.pdb
         {\tt cubane.pdb}
512
         cyclobutane.pdb
512
         cyclohexanol.pdb
512
         cyclopropane.pdb
         ethane.pdb
512
512
         ethanol.pdb
         ethylcyclohexane.pdb
glycol.pdb
heme.pdb
512
512
128K
512
         lactic-acid.pdb
512
         lactose.pdb
128K
         lanoxin.pdb
         lsd.pdb '
maltose.pdb
512
512
512
         menthol.pdb
512
         methane.pdb
         methanol.pdb
512
512
         mint.pdb
512
512
         morphine.pdb
         mustard.pdb
512
         nerol.pdb
512
         norethindrone.pdb
512
         octane.pdb
512
         pentane.pdb
512
512
         piperine.pdb
         propane.pdb
```

| 512 | pyridoxal.pdb      |
|-----|--------------------|
| 512 | quinine.pdb        |
| 512 | strychnine.pdb     |
| 512 | styrene.pdb        |
| 512 | sucrose.pdb        |
| 512 | testosterone.pdb   |
| 512 | thiamine.pdb       |
| 512 | tnt.pdb            |
| 512 | tuberin.pdb        |
| 512 | tyrian-purple.pdb  |
| 512 | vanillin.pdb       |
| 512 | vinyl-chloride.pdb |
| 512 | vitamin-a.pdb      |