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### PS5

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#### 1.1

```
[ese-maizl@login01 ~]$ ln data_demo data_demo_link
ln: 'data_demo': hard link not allowed for directory
[ese-maizl@login01 ~]$ ln -s data_demo data_demo_link
[ese-maizl@login01 ~]$ ll
total 4
drwxr-xr-x 8 ese-maizl ese-ouycc 4096 Dec 3 16:39 data_demo
                                          9 Dec
                                                     4 10:33 data_demo_link -> data_demo
1 20:27 err.log
lrwxrwxrwx 1 ese-maizl ese-ouycc
-rw-r--r-- 1 ese-maizl ese-ouycc
                                             0 Dec
drwxr-xr-x 2 ese-maizl ese-ouycc 4096 Nov
                                                      2 18:47 exam
-rw-r--r-- 1 ese-maizl ese-ouycc 3637 Dec
                                                      1 20:27 job.log
-rw-r--r-- 1 ese-maizl ese-ouycc 380 Dec
                                                     1 19:55 job.sh
                                                     3 17:55 mpi_demo
drwxr-xr-x 2 ese-maizl ese-ouycc 4096 Dec
-rw-r--r-- 1 ese-maizl ese-ouycc
                                          92 Dec
                                                     1 20:27 result.log
-rw-r--r-- 1 ese-maizl ese-ouycc 239 Dec
                                                     1 20:36 t1.py
```

## 1.2

```
[ese-maizl@login01 ~]$ pwd
/work/ese-maizl
[ese-maizl@login01 ~]$ echo $(pwd)
/work/ese-maizl
```

```
[ese-maizl@login01 molecules]$ ll
total 3
-rwxr-xr-x 1 ese-maizl ese-ouycc 1158 Nov 24 19:21 cubane.pdb
-rwxr-xr-x 1 ese-maizl ese-ouycc 622 Nov 24 19:21 ethane.pdb
-rwxr-xr-x 1 ese-maizl ese-ouycc 422 Nov 24 19:21 methane.pdb
-rwxr-xr-x 1 ese-maizl ese-ouycc 1828 Nov 24 19:21 octane.pdb
-rwxr-xr-x 1 ese-maizl ese-ouycc 1226 Nov 24 19:21 pentane.pdb
-rwxr-xr-x 1 ese-maizl ese-ouycc 825 Nov 24 19:21 propane.pdb
[ese-maizl@login01 molecules]$ touch test.pdb
[ese-maizl@login01 molecules]$ ll
total 3
-rwxr-xr-x 1 ese-maizl ese-ouycc 1158 Nov 24 19:21 cubane.pdb
-rwxr-xr-x 1 ese-maizl ese-ouycc 622 Nov 24 19:21 ethane.pdb
-rwxr-xr-x 1 ese-maizl ese-ouycc 422 Nov 24 19:21 methane.pdb
-rwxr-xr-x 1 ese-maizl ese-ouycc 1828 Nov 24 19:21 octane.pdb
-rwxr-xr-x 1 ese-maizl ese-ouycc 1226 Nov 24 19:21 pentane.pdb
-rwxr-xr-x 1 ese-maizl ese-ouycc 825 Nov 24 19:21 propane.pdb
-rw-r--r-- 1 ese-maizl ese-ouycc 0 Dec 4 10:52 test.pdb
```

```
[ese-maizl@login01 ~]$ find /work/ese-maizl/data_demo/data/elements/ -type f -print | wc -w 103
```

## 1.5

```
[ese-maizl@login01 pdb]$ diff ethane.pdb ethanol.pdb
1,11c1,12
< COMPND
               ETHANE
< AUTHOR
               DAVE WOODCOCK 95 12 18
< ATOM
< ATOM
< ATOM
                                   -0.752
                                               0.001 -0.141 1.00 0.00
            2 C
3 H
4 H
5 H
6 H
                                      0.752 -0.001 0.141 1.00 0.00
                                                       0.070 1.00 0.00
0.496 1.00 0.00
-1.188 1.00 0.00
-0.070 1.00 0.00
                                     -1.158 0.991
< ATOM
                                                       0.496
-1.188
                                     -1.240
                                              -0.737
                                             -0.249
                                     -0.924
< ATOM
                                     1.158 -0.991 -0.070
< ATOM
                                     0.924 0.249 1.188 1.00 0.00
< ATOM
                                      1.240 0.737 -0.496 1.00 0.00
             8 H
< ATOM
< TER
             9
> COMPND
             ETHANOL
                                     -0.599 1.244 -0.481 1.00 0.00

-0.750 -0.738 -0.981 1.00 0.00

-1.022 -0.351 0.30
> AUTHOR
               DAVE WOODCOCK 96 01 03
> ATOM
                                  -0.426 -0.115 -0.147
             2 0
3 H
> ATOM
> ATOM
                             1
             4 H
> ATOM
             5 H
                                              1.434 -0.689 1.00 0.00
> ATOM
                            1
> ATOM
             6 C
                                     1.047 -0.383 0.147 1.00 0.00
                                      1.370 0.240 0.981 1.00 0.00
> ATOM
             7 H
                                                       -0.735 1.00 0.00
0.405 1.00 0.00
             8 H
                                      1.642 -0.147
> ATOM
                                      1.180 -1.434
> ATOM
             9
                н
                              1
> TER
            10
```

```
[ese-maizl@login01 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-maizl@login01 data]$ du
665 ./pdb
52 ./elements
1 ./animal-counts
976 .
```

```
[ese-maizl@login01 data_demo]$ cp -r writting/ ./writting_new
[ese-maizl@login01 data_demo]$ ll
drwxr-xr-x 2 ese-maizl ese-ouycc 4096 Nov 24 19:21 creatures
drwxr-xr-x 5 ese-maizl ese-ouycc 4096 Nov 24 19:21 data
                                          100 Dec 3 16:40 log1
-rw-r--r-- 1 ese-maizl ese-ouycc
                                          200 Dec 3 16:39 log2
4096 Dec 4 10:52 molecules
4096 Nov 24 19:21 north-pacific-gyre
-rw-r--r-- 1 ese-maizl ese-ouycc
drwxr-xr-x 2 ese-maizl ese-ouycc
drwxr-xr-x 3 ese-maizl ese-ouycc
-rwxr-xr-x 1 ese-maizl ese-ouycc
                                             69 Nov 24 19:21 notes
                                              32 Nov 24 19:21 pizza.cfg
-rwxr-xr-x 1 ese-maizl ese-ouycc
-rwxr-xr-x 1 ese-maizl ese-ouycc 21583 Nov 24 19:21 solar.pdf
drwxr-xr-x 2 ese-maizl ese-ouycc 4096 Nov 24 20:19 test
drwxr-xr-x 5 ese-maizl ese-ouycc 4096 Nov 24 19:21 writting
drwxr-xr-x 5 ese-maizl ese-ouycc 4096 Dec 4 12:54 writting new
[ese-maizl@login01 data_demo]$ zip -q -r writting_new.zip ./writting_new/
[ese-maizl@login01 data_demo]$ ll
total 134
drwxr-xr-x 2 ese-maizl ese-ouycc
                                             4096 Nov 24 19:21 creatures
drwxr-xr-x 5 ese-maizl ese-ouycc
                                             4096 Nov 24 19:21 data
-rw-r--r-- 1 ese-maizl ese-ouycc
                                              100 Dec 3 16:40 log1
                                                         3 16:39 log2
-rw-r--r-- 1 ese-maizl ese-ouycc
                                              200 Dec
                                             4096 Dec 4 10:52 molecules
4096 Nov 24 19:21 north-pacific-gyre
drwxr-xr-x 2 ese-maizl ese-ouycc
drwxr-xr-x 3 ese-maizl ese-ouycc
                                                69 Nov 24 19:21 notes
-rwxr-xr-x 1 ese-maizl ese-ouycc
                                                32 Nov 24 19:21 pizza.cfg
-rwxr-xr-x 1 ese-maizl ese-ouycc
-rwxr-xr-x 1 ese-maizl ese-ouycc 21583 Nov 24 19:21 solar.pdf
                                            4096 Nov 24 20:19 test
4096 Nov 24 19:21 writting
drwxr-xr-x 2 ese-maizl ese-ouycc
drwxr-xr-x 5 ese-maizl ese-ouycc
drwxr-xr-x 5 ese-maizl ese-ouycc
drwxr-xr-x 5 ese-maizl ese-ouycc 4096 Dec 4 12:54 writting_new
-rw-r--r-- 1 ese-maizl ese-ouycc 422610 Dec 4 12:55 writting_new.zip
[ese-maizl@login01 data demo]$ unzip -q -o writting new.zip
[ese-maizl@login01 data_demo]$ ll
total 646
drwxr-xr-x 2 ese-maizl ese-ouycc
                                             4096 Nov 24 19:21 creatures
drwxr-xr-x 5 ese-maizl ese-ouycc
                                             4096 Nov 24 19:21 data
-rw-r--r-- 1 ese-maizl ese-ouvcc
                                             100 Dec
                                                         3 16:40 log1
                                              200 Dec
                                                         3 16:39 log2
-rw-r--r-- 1 ese-maizl ese-ouycc
                                             4096 Dec 4 10:52 molecules
4096 Nov 24 19:21 north-pacific-gyre
drwxr-xr-x 2 ese-maizl ese-ouycc
drwxr-xr-x 3 ese-maizl ese-ouycc
                                               69 Nov 24 19:21 notes
-rwxr-xr-x 1 ese-maizl ese-ouycc
-rwxr-xr-x 1 ese-maizl ese-ouycc
                                                32 Nov 24 19:21 pizza.cfg
-rwxr-xr-x 1 ese-maizl ese-ouycc
                                            21583 Nov 24 19:21 solar.pdf
drwxr-xr-x 2 ese-maizl ese-ouycc 4096 Nov 24 20:19 test
drwxr-xr-x 5 ese-maizl ese-ouycc 4096 Nov 24 19:21 writting
drwxr-xr-x 5 ese-maizl ese-ouycc 4096 Dec 4 12:56 writting_new
-rw-r--r-- 1 ese-maizl ese-ouycc 422610 Dec 4 12:55 writting_new.zip
```

```
[ese-maizl@login01 data_demo]$ ll
total 646
                                          4096 Nov 24 19:21 creatures
drwxr-xr-x 2 ese-maizl ese-ouycc
drwxr-xr-x 5 ese-maizl ese-ouycc
                                          4096 Nov 24 19:21 data
                                           100 Dec 3 16:40 log1
200 Dec 3 16:39 log2
4096 Dec 4 10:52 molecules
-rw-r--r-- 1 ese-maizl ese-ouycc
-rw-r--r-- 1 ese-maizl ese-ouycc
drwxr-xr-x 2 ese-maizl ese-ouycc
                                          4096 Dec
                                          4096 Nov 24 19:21 north-pacific-gyre
drwxr-xr-x 3 ese-maizl ese-ouycc
                                           69 Nov 24 19:21 notes
-rwxr-xr-x 1 ese-maizl ese-ouycc
                                            32 Nov 24 19:21 pizza.cfg
-rwxr-xr-x 1 ese-maizl ese-ouycc
-rwxr-xr-x 1 ese-maizl ese-ouycc 21583 Nov 24 19:21 solar.pdf
                                       4096 Nov 24 20:19 test
drwxr-xr-x 2 ese-maizl ese-ouycc
drwxr-xr-x 5 ese-maizl ese-ouycc
                                         4096 Nov 24 19:21 writting
                                         4096 Dec 4 12:56 writting_new
22610 Dec 4 12:55 writting_new.zip
d-wx--x--x 5 ese-maizl ese-ouycc 4096 Dec
-rw-r--r-- 1 ese-maizl ese-ouycc 422610 Dec
[ese-maizl@login01 data_demo]$ chmod 750 writting_new
[ese-maizl@login01 data_demo]$ ll
total 646
drwxr-xr-x 2 ese-maizl ese-ouycc
                                          4096 Nov 24 19:21 creatures
                                          4096 Nov 24 19:21 data
drwxr-xr-x 5 ese-maizl ese-ouycc
-rw-r--r-- 1 ese-maizl ese-ouycc
                                          100 Dec 3 16:40 log1
-rw-r--r-- 1 ese-maizl ese-ouycc
drwxr-xr-x 2 ese-maizl ese-ouycc
drwxr-xr-x 3 ese-maizl ese-ouycc
                                          200 Dec 3 16:39 log2
4096 Dec 4 10:52 molecules
4096 Nov 24 19:21 north-pacific-gyre
-rwxr-xr-x 1 ese-maizl ese-ouycc
                                            69 Nov 24 19:21 notes
-rwxr-xr-x 1 ese-maizl ese-ouycc
                                            32 Nov 24 19:21 pizza.cfg
-rwxr-xr-x 1 ese-maizl ese-ouvcc
                                       21583 Nov 24 19:21 solar.pdf
drwxr-xr-x 2 ese-maizl ese-ouycc
                                        4096 Nov 24 20:19 test
                                         4096 Nov 24 19:21 writting
drwxr-xr-x 5 ese-maizl ese-ouycc
drwxr-x--- 5 ese-maizl ese-ouycc
                                         4096 Dec 4 12:56 writting_new
-rw-r--r-- 1 ese-maizl ese-ouycc 422610 Dec 4 12:55 writting new.zip
```

```
[ese-maizl@login01 data_demo]$ history 10
624 pwd
625 man history
626 cd data_demo/data/
627 cd ..
628 cd writting
629 ll
630 cd .
631 cd ..
632 history |tail 10
633 history 10
```

```
GG Get Help O WriteOut R Read File Y Prev Page K Cut Text C Cur Pos X Exit J Justify Where Is V Next Page U UnCut Text To Spell
```

```
[ese-maizl@login01 pdb]$ ./printfile.sh
11193 /work/ese-maizl/data_demo/data/pdb/lanoxin.pdb
490
         /work/ese-maizl/data_demo/data/pdb/methanol.pdb
         /work/ese-maizl/data_demo/data/pdb/citronellal.pdb
1694
         /work/ese-maizl/data_demo/data/pdb/norethindrone.pdb
2729
4209
         /work/ese-maizl/data_demo/data/pdb/heme.pdb
2123
         /work/ese-maizl/data_demo/data/pdb/mustard.pdb
306
         /work/ese-maizl/data_demo/data/pdb/ammonia.pdb
1444
         /work/ese-maizl/data_demo/data/pdb/ascorbic-acid.pdb
1064
         /work/ese-maizl/data_demo/data/pdb/lactic-acid.pdb
422
         /work/ese-maizl/data_demo/data/pdb/methane.pdb
2288
         /work/ese-maizl/data_demo/data/pdb/morphine.pdb
2287
         /work/ese-maizl/data_demo/data/pdb/piperine.pdb
2562
         /work/ese-maizl/data_demo/data/pdb/maltose.pdb
2787
         /work/ese-maizl/data_demo/data/pdb/testosterone.pdb
         /work/ese-maizl/data_demo/data/pdb/testosterone.pdb
/work/ese-maizl/data_demo/data/pdb/thiamine.pdb
/work/ese-maizl/data_demo/data/pdb/tyrian-purple.pdb
/work/ese-maizl/data_demo/data/pdb/tuberin.pdb
2196
3303
2103
2395
         /work/ese-maizl/data_demo/data/pdb/cinnamaldehyde.pdb
1090
         /work/ese-maizl/data_demo/data/pdb/vitamin-a.pdb
2894
         /work/ese-maizl/data_demo/data/pdb/ethylcyclohexane.pdb
2396
         /work/ese-maizl/data_demo/data/pdb/strychnine.pdb
2675
2562
         /work/ese-maizl/data_demo/data/pdb/sucrose.pdb
1226
         /work/ese-maizl/data_demo/data/pdb/pentane.pdb
1680
         /work/ese-maizl/data_demo/data/pdb/nerol.pdb
423
         /work/ese-maizl/data_demo/data/pdb/vinyl-chloride.pdb
1830
         /work/ese-maizl/data_demo/data/pdb/camphene.pdb
1516
         /work/ese-maizl/data_demo/data/pdb/aldrin.pdb
1158
         /work/ese-maizl/data_demo/data/pdb/cubane.pdb
690
         /work/ese-maizl/data_demo/data/pdb/ethanol.pdb
         /work/ese-maizl/data_demo/data/pdb/cholesterol.pdb
/work/ese-maizl/data_demo/data/pdb/cyclobutane.pdb
/work/ese-maizl/data_demo/data/pdb/tnt.pdb
/work/ese-maizl/data_demo/data/pdb/vanillin.pdb
/work/ese-maizl/data_demo/data/pdb/mint.pdb
/work/ese-maizl/data_demo/data/pdb/pyridoxal.pdb
5049
895
1508
1361
1869
1256
         /work/ese-maizl/data_demo/data/pdb/ethane.pdb
622
         /work/ese-maizl/data_demo/data/pdb/benzaldehyde.pdb
1030
         /work/ese-maizl/data_demo/data/pdb/lsd.pdb
3395
825
         /work/ese-maizl/data_demo/data/pdb/propane.pdb
1384
         /work/ese-maizl/data_demo/data/pdb/cyclohexanol.pdb
765
         /work/ese-maizl/data_demo/data/pdb/glycol.pdb
2452
         /work/ese-maizl/data_demo/data/pdb/codeine.pdb
1159
         /work/ese-maizl/data_demo/data/pdb/styrene.pdb
695
         /work/ese-maizl/data_demo/data/pdb/cyclopropane.pdb
2164
         /work/ese-maizl/data_demo/data/pdb/menthol.pdb
1828
         /work/ese-maizl/data_demo/data/pdb/octane.pdb
2562
          /work/ese-maizl/data_demo/data/pdb/lactose.pdb
```