Assignment 05 简秋华 12132202

1.More Linux Commands

Answers:

1.1

```
[ese-jianqh@login03 ~]$ ln -s data_demo data_demo_link #创建data_demo的软链接文件 (symbolic link)
[ese-jianqh@login03 ~]$ ls #查看目录下的内容 data_demo_link err.log exam job.log job.sh mpi_demo result.log t1.py
```

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

1.2

```
[ese-jianqh@login03 ~]$ echo $(pwd) #pwd:print working directory
/work/ese-jianqh
```

```
[ese-jianqh@login03 ~]$ echo $(pwd)
/work/ese-jianqh
```

1.3

```
[ese-jianqh@login03 ~]$ cd data_demo/molecules/
[ese-jianqh@login03 molecules]$ touch test.pdb #使用指令"touch"时,如果指定的文件不存在,则将创建一个新的空白文件。
[ese-jianqh@login03 molecules]$ ls
cubane.pdb ethane.pdb methane.pdb octane.pdb pentane.pdb propane.pdb
test.pdb
```

```
[ese-jianqh@login03 ~]$ cd data_demo/molecules/
[ese-jianqh@login03 molecules]$ touch test.pdb
[ese-jianqh@login03 molecules]$ ls
cubane.pdb ethane.pdb methane.pdb octane.pdb pentane.pdb propane.pdb test.pdb
```

```
[ese-jianqh@login03 ~]$ cd data_demo/data/elements/
[ese-jianqh@login03 elements]$ find . -type f -print | wc -l #.表示当前目录; -type f:指定要搜索的文件类型为f, f表示查找所有常规文件; -print:打印文件绝对路径; wc -l 统计输出信息的行数。
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```

```
[ese-jianqh@login03 elements]$ cd ../pdb/
[ese-jianqh@login03 pdb]$ diff ethane.pdb ethanol.pdb
1,11c1,12
< COMPND
            ETHANE
< AUTHOR
            DAVE WOODCOCK 95 12 18
           1 C
< ATOM
                        1
                               -0.752
                                       0.001 -0.141 1.00 0.00
          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
< ATOM
           4
             Н
                        1
                               -1.240 -0.737
                                               0.496 1.00
                                                           0.00
           5 H
                        1
                               -0.924 -0.249 -1.188 1.00
< ATOM
                               1.158 -0.991 -0.070 1.00
< ATOM
           6 H
                         1
                                                           0.00
< ATOM
          7 H
                        1
                               0.924 0.249 1.188 1.00 0.00
                                1.240 0.737 -0.496 1.00 0.00
          8 H
                        1
< ATOM
           9
                         1
< TFR
> COMPND
            ETHANOL
> AUTHOR
           DAVE WOODCOCK 96 01 03
                   1
           1 C
                               -0.426 -0.115 -0.147 1.00 0.00
> ATOM
> ATOM
           2 0
                        1
                               -0.599
                                      1.244 -0.481 1.00
                                                           0.00
          3 H
                               -0.750 -0.738 -0.981 1.00
> ATOM
                        1
> ATOM
          4
             Н
                        1
                               -1.022 -0.351
                                              0.735 1.00
                                                           0.00
           5 H
> ATOM
                        1
                               -1.642 1.434 -0.689 1.00
                                                           0.00
           6 C
                        1
                                1.047 -0.383
                                             0.147 1.00 0.00
> ATOM
           7
                        1
                                1.370 0.240
                                             0.981 1.00
                                                           0.00
> ATOM
             Н
> ATOM
           8 H
                        1
                                1.642 -0.147 -0.735 1.00
                                                           0.00
> ATOM
           9
                         1
                                1.180 -1.434
                                             0.405 1.00
                                                           0.00
```

```
[ese-jianqh@login03 elements]$ cd ../pdb/
[ese-jianqh@login03 pdb]$ diff ethane.pdb ethanol.pdb
< COMPND
              ETHANE
< AUTHOR
              DAVE WOODCOCK 95 12 18
                                 -0.752
< ATOM
            1 C
                                          0.001
                                                 -0.141 1.00
                                                                0.00
< ATOM
            2
                                  0.752 - 0.001
                                                  0.141 1.00
                                                                0.00
                                  -1.158 0.991
                                                  0.070 1.00
< ATOM
                                                                0.00
                                                         1.00
                                  -1.240 -0.737
                                                  0.496
< ATOM
                                                                0.00
                                 -0.924 -0.249
1.158 -0.991
0.924 0.249
                                                  -1.188
                                                          1.00
                          1
< ATOM
            5
                                                                0.00
                                                          1.00
1.00
            6
< ATOM
              Н
                           1
                                                  -0.070
                                                                0.00
                                                  1.188
< ATOM
            7
              Н
                           1
                                                                0.00
                                  1.240 0.737
                                                 -0.496 1.00
            8
< ATOM
              Н
                                                                0.00
< TER
            9
> COMPND
              ETHANOL
              DAVE WOODCOCK 96 01 03
> AUTHOR
                                 -0.426 -0.115
                                                  -0.147
> ATOM
                                                         1.00
                                                                0.00
                                                  -0.481
                                                         1.00
> ATOM
            2
                                  -0.599
                                          1.244
                                                                0.00
                                                          1.00
            3
                                  -0.750
                                                  -0.981
 ATOM
              Н
                           1
                                          -0.738
                                                                0.00
  ATOM
            4
                                  -1.022
                                          -0.351
                                                   0.735
                                                          1.00
                                                                0.00
            5
                           1
                                  -1.642
                                          1.434
                                                  -0.689
 MOTA
              Н
                                                          1.00
                                                                0.00
                                                   0.147
            6
                                   1.047
                                          -0.383
                                                          1.00
 ATOM
              С
                                                                0.00
 MOTA
              Н
                                  1.370
                                          0.240
                                                  0.981
                                                          1.00
                                                                0.00
                           1
 MOTA
                                  1.642 -0.147
                                                  -0.735
                                                          1.00
                                                                0.00
 MOTA
            9
                                   1.180 -1.434
                                                   0.405 1.00
                                                                0.00
           10
 TER
```

```
[ese-jianqh@login03 pdb]$ cd ~/data_demo/writing/data/
[ese-jianqh@login03 data]$ ls
LittleWomen.txt one.txt two.txt
[ese-jianqh@login03 data]$ grep -c "But she" LittleWomen.txt
15
```

```
[ese-jianqh@login03 pdb]$ cd ~/data_demo/writing/data/
[ese-jianqh@login03 data]$ ls
LittleWomen.txt one.txt two.txt
[ese-jianqh@login03 data]$ grep -c "But she" LittleWomen.txt
15
```

1.7

```
[ese-jianqh@login03 data]$ cd ~/data_demo/data/
[ese-jianqh@login03 data]$ ls
amino-acids.txt animal-counts animals.txt elements morse.txt pdb
planets.txt salmon.txt sunspot.txt
[ese-jianqh@login03 data]$ du -ch #c表示除了显示个别目录或文件的大小外,同时也显示所有目录或文件的总和; 以K, M, G为单位,提高信息的可读性。
537K ./pdb
52K ./elements
1.0K ./animal-counts
848K .
848K total
```

```
[ese-jianqh@login03 data]$ cd ~/data_demo/data/
[ese-jianqh@login03 data]$ ls
amino-acids.txt animal-counts animals.txt elements morse.txt pdb planets.txt salmon.txt sunspot.txt
[ese-jianqh@login03 data]$ du -ch
537K ./pdb
52K ./elements
1.0K ./animal-counts
848K .
848K total
```

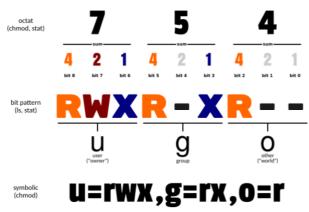
```
[ese-jianqh@login03 data]$ cd ..
[ese-jianqh@login03 data_demo]$ ls
creatures data log1 molecules my_file north-pacific-gyre notes pizza.cfg
solar.pdf test writing
[ese-jianqh@login03 data_demo]$ cp -r writing writing_new
[ese-jianqh@login03 data_demo]$ ls
creatures data log1 molecules my_file north-pacific-gyre notes pizza.cfg
solar.pdf test writing writing_new

[ese-jianqh@login03 data_demo]$ zip -q -m -r writing_new.zip writing_new #-q:不显
示指令执行过程; -m:将文件压缩并加入压缩文件后,删除原始文件,即把文件移到压缩文件中; -r: 递归处
理,将指定目录下的所有文件和子目录一并处理。
[ese-jianqh@login03 data_demo]$ ls
creatures data log1 molecules my_file north-pacific-gyre notes pizza.cfg
solar.pdf test writing writing_new.zip

[ese-jianqh@login03 data_demo]$ unzip writing_new.zip
```

```
Archive: writing_new.zip
     creating: writing_new/
    inflating: writing_new/haiku.txt
     creating: writing_new/tools/
   extracting: writing_new/tools/stats
     creating: writing_new/tools/old/
   extracting: writing_new/tools/old/oldtool
    inflating: writing_new/tools/format
     creating: writing_new/data/
    inflating: writing_new/data/one.txt
    inflating: writing_new/data/LittleWomen.txt
    inflating: writing_new/data/two.txt
     creating: writing_new/thesis/
   extracting: writing_new/thesis/empty-draft.md
  [ese-jianqh@login03 data_demo]$ ls
  creatures data log1 molecules my_file north-pacific-gyre notes pizza.cfg
   solar.pdf test writing writing_new writing_new.zip
[ese-jianqh@login03 data]$ cd ..
[ese-jianqh@login03 data_demo]$ ls
reatures data log1 molecules my_file north-pacific-gyre notes pizza.cfg solar.pdf test writing
[ese-jianqh@login03 data_demo]$ cp -r writing writing_new
[ese-jianqh@login03 data_demo]$ ls
        data log1 molecules my_file north-pacific-gyre notes pizza.cfg solar.pdf test writing writing_new
[ese-jianqh@login03 data_demo]$ zip -q -m -r writing_new.zip writing_new
[ese-jianqh@login03 data_demo]$ ls
creatures data loq1 molecules my file north-pacific-gyre notes piz
                             my file north
```

```
[ese-jianqh@login03 data demo]$ chmod 750 writing new
[ese-jianqh@login03 data_demo]$ ll
total 773
drwxr-xr-x 2 ese-jianqh ese-ouycc
                                      4096 Nov 24 19:21 creatures
drwxr-xr-x 5 ese-jiangh ese-ouycc
                                      4096 Dec 3 16:42 data
-rw-r--r-- 1 ese-jiangh ese-ouycc 10448 Dec
                                                3 16:43 log1
drwxr-xr-x 2 ese-jianqh ese-ouycc
                                      4096 Dec 8 14:12 molecules
                                        68 Nov 24 19:56 my_file
-rw-r--r-- 1 ese-jianqh ese-ouycc
drwxr-xr-x 3 ese-jianqh ese-ouycc
-rwxr-xr-x 1 ese-jianqh ese-ouycc
-rwxr-xr-x 1 ese-jianqh ese-ouycc
                                      4096 Nov 24 19:21 north-pacific-gyre
                                         69 Nov 24 19:21 notes
                                         32 Nov 24 19:21 pizza.cfg
-rwxr-xr-x 1 ese-jiangh ese-ouycc 21583 Nov 24 19:21 solar.pdf
drwxr-xr-x 2 ese-jianqh ese-ouycc
                                      4096 Nov 24 19:56 test
drwxr-xr-x 5 ese-jiangh ese-ouycc
                                      4096 Nov 24 19:21 writing
drwxr-x--- 5 ese-jiangh ese-ouycc
                                      4096 Dec 8 15:07 writing new
-rw-r--r-- 1 ese-jiangh ese-ouycc 422584 Dec 8 15:13 writing new.zip
```



Picture from: https://www.runoob.com/linux/linux-comm-chmod.html

```
[ese-jianqh@login03 data_demo]$ history 10
346 ls
347 cd ..
348 ls
349 zip -q -m -r writing_new.zip writing_new
350 ls
351 unzip writing_new.zip
352 ls
353 chmod 750 writing_new
354 ll
355 history 10
```

```
[ese-jianqh@login03 data demo]$ history 10
  346
      ls
  347
      cd ..
 348
      ls
       zip -q -m -r writing new.zip writing new
 349
  350
      ls
  351
      unzip writing_new.zip
 352
  353
      chmod 750 writing new
  354
      ш
  355
     history 10
```

2.BASH for loop

Answers:

```
[ese-jianqh@login03 pdb]$ nano pd.sh
[ese-jianqh@login03 pdb]$ bash pd.sh
1.5K aldrin.pdb
306 ammonia.pdb
1.5K ascorbic-acid.pdb
1.1K benzaldehyde.pdb
1.8K camphene.pdb
5.0K cholesterol.pdb
1.1K cinnamaldehyde.pdb
1.7K citronellal.pdb
2.4K codeine.pdb
1.2K cubane.pdb
895 cyclobutane.pdb
1.4K cyclohexanol.pdb
695 cyclopropane.pdb
622 ethane.pdb
690 ethanol.pdb
2.4K ethylcyclohexane.pdb
765 glycol.pdb
4.2K heme.pdb
1.1K lactic-acid.pdb
2.6K lactose.pdb
11K lanoxin.pdb
3.4K lsd.pdb
2.6K maltose.pdb
2.2K menthol.pdb
422 methane.pdb
490 methanol.pdb
1.9K mint.pdb
2.3K morphine.pdb
2.1K mustard.pdb
1.7K nerol.pdb
2.7K norethindrone.pdb
1.8K octane.pdb
1.2K pentane.pdb
2.3K piperine.pdb
825 propane.pdb
1.3K pyridoxal.pdb
3.3K quinine.pdb
2.7K strychnine.pdb
1.2K styrene.pdb
2.6K sucrose.pdb
2.8K testosterone.pdb
2.2K thiamine.pdb
1.5K tnt.pdb
2.4K tuberin.pdb
2.1K tyrian-purple.pdb
1.4K vanillin.pdb
423 vinyl-chloride.pdb
2.9K vitamin-a.pdb
#pd.sh
for file in *.pdb
do
```

```
echo $(du -bh $file) #
done
```

```
for thing in *.pdb
do
    echo $(du -bh $file)
done
```

```
[ese-jianqh@login03 pdb]$ nano pd.sh
[ese-jianqh@login03 pdb]$ bash pd.sh
1.5K aldrin.pdb
306 ammonia.pdb
1.5K ascorbic-acid.pdb
1.1K benzaldehyde.pdb
1.8K camphene.pdb
5.0K cholesterol.pdb
1.1K cinnamaldehyde.pdb
1.7K citronellal.pdb
2.4K codeine.pdb
1.2K cubane.pdb
895 cyclobutane.pdb
1.4K cyclohexanol.pdb
695 cyclopropane.pdb
622 ethane.pdb
690 ethanol.pdb
2.4K ethylcyclohexane.pdb
765 glycol.pdb
4.2K heme.pdb
1.1K lactic-acid.pdb
2.6K lactose.pdb
11K lanoxin.pdb
3.4K lsd.pdb
2.6K maltose.pdb
2.2K menthol.pdb
422 methane.pdb
490 methanol.pdb
1.9K mint.pdb
2.3K morphine.pdb
2.1K mustard.pdb
1.7K nerol.pdb
2.7K norethindrone.pdb
1.8K octane.pdb
1.2K pentane.pdb
2.3K piperine.pdb
825 propane.pdb
1.3K pyridoxal.pdb
3.3K quinine.pdb
2.7K strychnine.pdb
1.2K styrene.pdb
2.6K sucrose.pdb
2.8K testosterone.pdb
2.2K thiamine.pdb
1.5K tnt.pdb
2.4K tuberin.pdb
2.1K tyrian-purple.pdb
1.4K vanillin.pdb
423 vinyl-chloride.pdb
2.9K vitamin-a.pdb
```