

Assignment 05 简秋华 12132202

Good job and clear report!

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 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
```

1.4

```
[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。
103
```

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

1.5

```
[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
< 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
```

```
[ese-jianqh@login03 elements]$ cd ../pdb/
[ese-jianqh@login03 pdb]$ diff ethane.pdb ethanol.pdb
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< 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-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
```

1.8

```
[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_demo]$ 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
[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

```

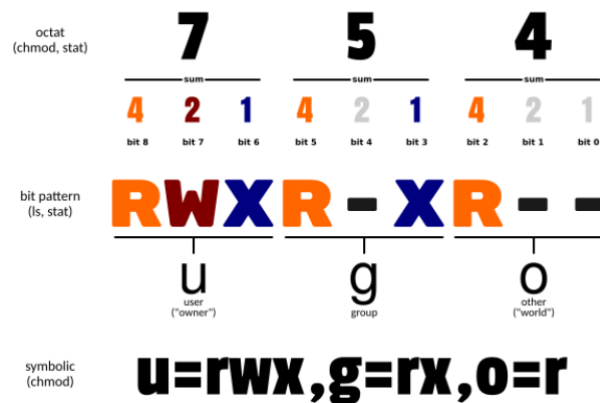
1.9

```

[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-jianqh ese-ouycc 4096 Dec  3 16:42 data
-rw-r--r-- 1 ese-jianqh ese-ouycc 10448 Dec  3 16:43 log1
drwxr-xr-x 2 ese-jianqh ese-ouycc 4096 Dec  8 14:12 molecules
-rw-r--r-- 1 ese-jianqh ese-ouycc 68 Nov 24 19:56 my_file
drwxr-xr-x 3 ese-jianqh ese-ouycc 4096 Nov 24 19:21 north-pacific-gyre
-rwxr-xr-x 1 ese-jianqh ese-ouycc 69 Nov 24 19:21 notes
-rwxr-xr-x 1 ese-jianqh ese-ouycc 32 Nov 24 19:21 pizza.cfg
-rwxr-xr-x 1 ese-jianqh 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-jianqh ese-ouycc 4096 Nov 24 19:21 writing
drwxr-x--- 5 ese-jianqh ese-ouycc 4096 Dec  8 15:07 writing_new #The result
-rw-r--r-- 1 ese-jianqh ese-ouycc 422584 Dec  8 15:13 writing_new.zip

```

```
[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-jianqh ese-ouycc 4096 Dec  3 16:42 data
-rw-r--r-- 1 ese-jianqh ese-ouycc 10448 Dec  3 16:43 log1
drwxr-xr-x 2 ese-jianqh ese-ouycc 4096 Dec  8 14:12 molecules
-rw-r--r-- 1 ese-jianqh ese-ouycc 68 Nov 24 19:56 my_file
drwxr-xr-x 3 ese-jianqh ese-ouycc 4096 Nov 24 19:21 north-pacific-gyre
-rwxr-xr-x 1 ese-jianqh ese-ouycc 69 Nov 24 19:21 notes
-rwxr-xr-x 1 ese-jianqh ese-ouycc 32 Nov 24 19:21 pizza.cfg
-rwxr-xr-x 1 ese-jianqh 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-jianqh ese-ouycc 4096 Nov 24 19:21 writing
drwxr-x-- 5 ese-jianqh ese-ouycc 4096 Dec  8 15:07 writing_new
-rw-r--r-- 1 ese-jianqh ese-ouycc 422584 Dec  8 15:13 writing_new.zip
```



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

1.10

```
[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
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
```

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 citronella.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
```