

Assignment 05

Good job!

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1. More Linux Commands

In this exercise, we will learn a few more Linux commands. For each command, please use `man` to learn what it does and how to use it correctly. First, change your directory to `~`.

```
[ese-gongggq@login02 ~]$ ls
data_demo  err.log  exam  job.sh  mpi_demo  result.log  t1.py
```

1.1 [2 points] Make a link called `data_demo_link` to `data_demo` folder using `ln`.

```
[ese-gongggq@login02 ~]$ ln -s data_demo data_demo_link
[ese-gongggq@login02 ~]$ ls
data_demo  data_demo_link  err.log  exam  job.sh  mpi_demo  result.log  t1.py
```

1.2 [2 points] Print your home directory using `echo`.

```
[ese-gongggq@login02 ~]$ echo $HOME
/work/ese-gongggq
```

1.3 [2 points] Go to `data_demo/molecules/`, make an empty file `test.pdb` with `touch`.

```
[ese-gongggq@login02 ~]$ cd data_demo/molecules/
[ese-gongggq@login02 molecules]$ touch test.pdb
[ese-gongggq@login02 molecules]$ ls
cubane.pdb  methane.pdb  pentane.pdb  test.pdb
ethane.pdb  octane.pdb   propane.pdb
```

1.4 [3 points] Find how many files in `data_demo/data/elements/` using `find`.

```
[ese-gongggq@login02 ~]$ find data_demo/data/elements/ -name "*" | wc -l
103
```

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1.5 [2 points] Compare data_demo/data/pdb/ethane.pdb and data_demo/data/pdb/ethanol.pdb with diff.

```
[ese-gongggq@login02 ~]$ diff data_demo/data/pdb/ethane.pdb data_demo/data/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 [3 points] Count how many But she string appears in data_demo/writing/data/LittleWomen.txt with grep.

```
[ese-gongggq@login02 ~]$ grep "But she" data_demo/writing/data/LittleWomen.txt -o | wc -l
15
```

1.7 [2 points] Check the total file size of the data_demo/data/ folder using du.

```
[ese-gongggq@login02 ~]$ du data_demo/data/ -c
409    data_demo/data/pdb
52     data_demo/data/elements
1      data_demo/data/animal-counts
720    data_demo/data/
720    总用量
```

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- 1.8 [3 points]** Copy the `data_demo/writing/` folder to `data_demo/writing_new/`,
compress `data_demo/writing_new/` using `zip`, and decompress the `.zip` file with `unzip`.

```
[ese-gongggq@login02 ~]$ cp -f -r data_demo/writing data_demo/writing_new/
[ese-gongggq@login02 ~]$ cp data_demo/
cp: 在 "data_demo" 后缺少了要操作的目标文件
Try 'cp --help' for more information.
[ese-gongggq@login02 ~]$ cp data_demo/
cp: 在 "data_demo/" 后缺少了要操作的目标文件
Try 'cp --help' for more information.
[ese-gongggq@login02 ~]$ cd data_demo
[ese-gongggq@login02 data_demo]$ ls
creatures  data  log1  log2  molecules  north-pacific-gyre  notes  pizza.cfg  solar.pdf  writing  writing_new
```

```
[ese-gongggq@login02 data_demo]$ zip -r -q zipfile.zip writing_new
[ese-gongggq@login02 data_demo]$ ls
creatures  log1  molecules  notes  solar.pdf  writing_new
data       log2  north-pacific-gyre  pizza.cfg  writing  zipfile.zip
[ese-gongggq@login02 data_demo]$ rm -r writing_new
[ese-gongggq@login02 data_demo]$ ls
creatures  data  log1  log2  molecules  north-pacific-gyre  notes  pizza.cfg  solar.pdf  writing  zipfile.zip
```

```
[ese-gongggq@login02 data_demo]$ unzip -q zipfile.zip
[ese-gongggq@login02 data_demo]$ ls
creatures  log1  molecules  notes  solar.pdf  writing_new
data       log2  north-pacific-gyre  pizza.cfg  writing  zipfile.zip
```

- 1.9 [3 points]** Change the file permissions flags on `writing_new` to `drwxr-x---` using `chmod`.

```
[ese-gongggq@login02 data_demo]$ chmod 750 writing_new/
[ese-gongggq@login02 data_demo]$ ll
总用量 645
drwxr-xr-x 2 ese-gongggq ese-ouycc 4096 11月 24 19:18 creatures
drwxr-xr-x 5 ese-gongggq ese-ouycc 4096 11月 24 19:18 data
-rw-r--r-- 1 ese-gongggq ese-ouycc 0 12月 3 16:34 log1
-rw-r--r-- 1 ese-gongggq ese-ouycc 100 12月 3 16:33 log2
drwxr-xr-x 2 ese-gongggq ese-ouycc 4096 12月 7 08:37 molecules
drwxr-xr-x 3 ese-gongggq ese-ouycc 4096 11月 24 19:18 north-pacific-gyre
-rwxr-xr-x 1 ese-gongggq ese-ouycc 69 11月 24 19:52 notes
-rwxr-xr-x 1 ese-gongggq ese-ouycc 32 11月 24 19:52 pizza.cfg
-rwxr-xr-x 1 ese-gongggq ese-ouycc 21583 11月 24 19:52 solar.pdf
drwxr-xr-x 5 ese-gongggq ese-ouycc 4096 11月 24 19:18 writing
drwxr-x--- 5 ese-gongggq ese-ouycc 4096 12月 7 09:13 writing_new
-rw-r--r-- 1 ese-gongggq ese-ouycc 422584 12月 7 09:15 zipfile.zip
```

- 1.10 [3 points]** Print the last 10 commands you made using `history`

```
[ese-gongggq@login02 data_demo]$ history | tail -10
278  ls
279  rm -r writing_new
280  ls
281  unzip -q zipfile.zip
282  ls
283  chmod 750 writing_new/
284  ll
285  history | tali -10
286  history | tail-10
287  history | tail -10
[ese-gongggq@login02 data_demo]$
```

2. BASH for Loop

The general syntax of a BASH loop goes like:

```
for thing in list_of_things
do
    operation_using $thing
done
```

[5 points] Write a shell script to print file size (in bytes) of each *.pdb file in data_demo/data/pdb/, line by line.

```
[ese-gongggq@login02 ~]$ vi loop.sh
```

```
ssh
for file in data_demo/data/pdb/*.pdb
do
    du -b $file
done
```

```

[ese-gonggq@login02 ~]$ ls
data_demo      err.log      job.sh      mpi_demo    t1.py
data_demo_link exam         loop.sh     result.log

[ese-gonggq@login02 ~]$ ./loop.sh
1516  data_demo/data/pdb/aldrin.pdb
306   data_demo/data/pdb/ammonia.pdb
1444  data_demo/data/pdb/ascorbic-acid.pdb
1030  data_demo/data/pdb/benzaldehyde.pdb
1830  data_demo/data/pdb/camphene.pdb
5049  data_demo/data/pdb/cholesterol.pdb
1090  data_demo/data/pdb/cinnamaldehyde.pdb
1694  data_demo/data/pdb/citronellal.pdb

```

loop.sh code reference to chen penghan
thanks penghan

Clear reference