

Assignment 5

本节学习了 Linux 操作系统,学习了 Linux 操作指令。首先是通过 [ssh](#) 远程访问太乙账号 [ese-zhangchjy@172.18.6.175](#)

```
ngchjy@172.18.6.175
ese-zhangchjy@172.18.6.175's password:
Last login: Fri Dec 3 16:44:27 2021 from 172.18.6.68
Welcome to the SUSTech HPC

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QUEUE'S RUNLIMIT NOTICE.
debug: 20 min less than 80c Open
ser: 168h Unlimited Open
short: 168h More Than 40c Open
medium: 168h More Than 200c Open
large: 72h More Than 600c Open
smp: 168h Unlimited Open
gpu: 168h Unlimited Open

User--guide: http://hpc.sustech.edu.cn/process/user_guide.html
login ip: 172.18.6.175

CCSE WeChat public account : gh_7cd85ddedaf7
Support Team QQ: 161195492
Support Team Email: hpc@sustech.edu.cn
Support Team Phone: 0755-88015831,17318031826, 1598664

Attention:
1. Please do not run jobs that keep generating numerous files for a long time before contacting the support team for a proper solution, because it will cause a high pressure to the storage system and slow down everyone.
2. Please do not run large memory jobs on the login node because it will slow down everyone.
3. Please do not use MPI in job, because it may cause high pressure to the storage system and slow down everyone.
4. In order to ensure the security of data, please back up your data to your local disk regularly.

Warning: violation of the above rules may result in job termination and account blocking

BASIC COMMAND:
bsub < jobscript.bsub #submit a job
do not forget the '<'
bjobs #check the status of your jobs
bkill $JOBID1 $JOBID2 $JOBID3 #stop your jobs
ID1 ID2 ID3 ...
bhosts hg_short #check the status of queue short
us of queue short, you can check debug ser short medium

We strongly recommend the users to use the Issue Tracking system, when you have any problems in using the supercomputers of CCSE.
1. Address: http://172.18.6.195:18090/.
2. User Guide: https://hpc.sustech.edu.cn/ref/HPMS_UserGuide.pdf.
3. Customer Service Phone Number: 0755-88015833.

[ese-zhangchjy@login03 ~]$
```

首先我们要知道 man 指令可以查询 Linux 的命令使用方法

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

```
[ese-zhangchjy@login03 ~]$ ls
data_demo      exam      mpi_demo    t1.py
data_demo_link job.log   print.sh    t2.py
err.log        job.sh    result.log
```

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

```
[ese-zhangchjy@login03 ~]$ echo $HOME
/work/ese-zhangchjy
```

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

```
[ese-zhangchjy@login03 ~]$ cd data_demo/molecules/
[ese-zhangchjy@login03 molecules]$ touch test.pdb
[ese-zhangchjy@login03 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-zhangchjy@login03 ~]$ find data_demo/data/elements/ -name "*.*)" | wc -l
103
```

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

```
[ese-zhangchjy@login03 ~]$ 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-zhangchjy@login03 ~]$ 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-zhangchjy@login03 ~]$ du data_demo/data/ -c
408      data_demo/data/pdb
52       data_demo/data/elements
1        data_demo/data/animal-counts
720      data_demo/data/
720      总用量
```

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-zhangchjy@login03 ~]$ cp -rf data_demo/writing data_demo/writing_new/
[ese-zhangchjy@login03 ~]$ cd data_demo
[ese-zhangchjy@login03 data_demo]$ ls
creatures  log2      north-pacific-gyre  solar.pdf  writing_new
data       log1      notes               test       writing
log1       molecules pizza.cfg           writing
```

```
[ese-zhangchjy@login03 data_demo]$ zip -rq zipfile.zip writing_new/
[ese-zhangchjy@login03 data_demo]$ ls
creatures  log2      north-pacific-gyre  solar.pdf  writing_new
data       log1      notes               test       zipfile.zip
log1       molecules pizza.cfg           writing
[ese-zhangchjy@login03 data_demo]$ rm -r writing_new/
[ese-zhangchjy@login03 data_demo]$ ls
creatures  log2      north-pacific-gyre  solar.pdf  zipfile.zip
data       log1      notes               test
log1       molecules pizza.cfg           writing
```

```
[ese-zhangchjy@login03 data_demo]$ unzip -q zipfile.zip
[ese-zhangchjy@login03 data_demo]$ ls
creatures  log2      north-pacific-gyre  solar.pdf  writing_new
data       log1      notes               test       zipfile.zip
log1       molecules pizza.cfg           writing
```

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

```
[ese-zhangchjy@login03 data_demo]$ chmod 750 writing_new/
[ese-zhangchjy@login03 data_demo]$ ll
总用量 646
drwxr-xr-x 2 ese-zhangchjy ese-ouycc 4096 11月 24 19:23 creatures
drwxr-xr-x 5 ese-zhangchjy ese-ouycc 4096 11月 24 19:23 data
-rw-r--r-- 1 ese-zhangchjy ese-ouycc 636 12月 3 16:40 log1
-rw-r--r-- 1 ese-zhangchjy ese-ouycc 300 12月 3 16:34 log2
-rw-r--r-- 1 ese-zhangchjy ese-ouycc 100 12月 3 16:33 logl
drwxr-xr-x 2 ese-zhangchjy ese-ouycc 4096 12月 7 21:23 molecules
drwxr-xr-x 3 ese-zhangchjy ese-ouycc 4096 11月 24 19:23 north-pacific-
gyre
-rwxr-xr-x 1 ese-zhangchjy ese-ouycc 69 11月 24 19:24 notes
-rwxr-xr-x 1 ese-zhangchjy ese-ouycc 32 11月 24 19:24 pizza.cfg
-rwxr-xr-x 1 ese-zhangchjy ese-ouycc 21583 11月 24 19:24 solar.pdf
drwxr-xr-x 2 ese-zhangchjy ese-ouycc 4096 11月 24 19:52 test
drwxr-xr-x 5 ese-zhangchjy ese-ouycc 4096 11月 24 19:23 writing
drwxr-x--- 5 ese-zhangchjy ese-ouycc 4096 12月 7 21:40 writing_new
-rw-r--r-- 1 ese-zhangchjy ese-ouycc 422584 12月 7 21:42 zipfile.zip
```

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

```
[ese-zhangchjy@login03 data_demo]$ history | tail -10
247  ls
248  zip -rq zipfile.zip writing_new/
249  ls
250  rm -r writing_new/
251  ls
252  unzip -q zipfile.zip
253  ls
254  chmod 750 writing_new/
255  ll
256  history | tail -10
```

2. BASH for Loop

[5分]编写 shell 脚本，逐行打印 data_demo/data/pdb/中每个*.pdb 文件的文件大小（以字节为单位）

```
[ese-zhangchjy@login03 ~]$ nano loop.sh
[ese-zhangchjy@login03 ~]$ chmod 750 loop.sh
[ese-zhangchjy@login03 ~]$ ./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
2452 data_demo/data/pdb/codeine.pdb
1158 data_demo/data/pdb/cubane.pdb
895 data_demo/data/pdb/cyclobutane.pdb
1384 data_demo/data/pdb/cyclohexanol.pdb
695 data_demo/data/pdb/cyclopropane.pdb
622 data_demo/data/pdb/ethane.pdb
690 data_demo/data/pdb/ethanol.pdb
2396 data_demo/data/pdb/ethylcyclohexane.pdb
765 data_demo/data/pdb/glycol.pdb
4209 data_demo/data/pdb/heme.pdb
1064 data_demo/data/pdb/lactic-acid.pdb
2562 data_demo/data/pdb/lactose.pdb
11193 data_demo/data/pdb/lanoxin.pdb
3395 data_demo/data/pdb/lsd.pdb
2562 data_demo/data/pdb/maltose.pdb
2164 data_demo/data/pdb/menthol.pdb
422 data_demo/data/pdb/methane.pdb
490 data_demo/data/pdb/methanol.pdb
1869 data_demo/data/pdb/mint.pdb
2288 data_demo/data/pdb/morphine.pdb
2123 data_demo/data/pdb/mustard.pdb
1680 data_demo/data/pdb/nerol.pdb
2729 data_demo/data/pdb/norethindrone.pdb
1828 data_demo/data/pdb/octane.pdb
1226 data_demo/data/pdb/pentane.pdb
2287 data_demo/data/pdb/piperine.pdb
825 data_demo/data/pdb/propane.pdb
1256 data_demo/data/pdb/pyridoxal.pdb
3303 data_demo/data/pdb/quinine.pdb
2675 data_demo/data/pdb/strychnine.pdb
1159 data_demo/data/pdb/styrene.pdb
2562 data_demo/data/pdb/sucrose.pdb
2787 data_demo/data/pdb/testosterone.pdb
2196 data_demo/data/pdb/thiamine.pdb
```