ZHAO Ang (赵昂)'s TA report for assignment05

SID: 12132606

Github: https://github.com/ZINSIST/ESE5023_Assignments_12132606

Responsible TA: HUANG Hao

Grade: 30

1.1 Well done!

```
[ese-zhaoan@login01 ~]$ ln -s data_demo data_demo_link
[ese-zhaoan@login01 ~]$ ls
data_demo  data_demo_link  exam
[ese-zhaoan@login01 ~]$
```

1.2

```
[ese-zhaoan@login01 ~]$ echo *
data_demo data_demo_link exam
[ese-zhaoan@login01 ~]$
```

1.3

```
[ese-zhaoan@login01 molecules]$ touch test.pdb
[ese-zhaoan@login01 molecules]$ ls
cubane.pdb  ethane.pdb  methane.pdb  octane.pdb  pentane.pdb  propane.pdb  test.pdb
[ese-zhaoan@login01 molecules]$
```

1.4

```
./Cr.xml
./Rn.xml
./Ge.xml
./Co.xml
./Tc.xml
./Pm.xml
./Rb.xml
./C.xml
./Yb.xml
./Zn.xml
./Cs.xml
./Fm.xml
./Ni.xml
./Ar.xml
[ese-zhaoan@login01 elements]$ find . -type f -print | wc -l
103
```

1.5

```
[ese-zhaoan@login01 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              1
---
> 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
[ese-zhaoan@login01 pdb]$
```

1.6

```
LittleWomen.txt:15
[ese-zhaoan@login01 data]$ grep -c 'But she'  LittleWomen.txt
15
[ese-zhaoan@login01 data]$
```

1.7

```
[ese-zhaoan@login01 data]$ du -h
407K    ./pdb
52K     ./elements
1.0K    ./animal-counts
1.1M    .
```

1.8

```
[ese-zhaoan@login01 data_demo]$ cp -r writing writing_new
[ese-zhaoan@login01 data_demo]$ ls
creatures  data  draft.txt  molecules  north-pacific-gyre  notes  pizza.cfg  solar.pdf  thesis  writing  writing_new
[ese-zhaoan@login01 data_demo]$
```

```
[ese-zhaoan@login01 data_demo]$ zip writing_new.zip writing_new
  adding: writing_new/ (stored 0%)
[ese-zhaoan@login01 data_demo]$
```

```
[ese-zhaoan@login01 data_demo]$ unzip writing_new.zip
Archive:  writing_new.zip
[ese-zhaoan@login01 data_demo]$
baXterm by subscribing to the professional edition here:  https://mobaxterm.mobatek.net
```

1.9 Using 'chmod 750 data_demo/writing_new/' would be clean

```
[ese-zhaoan@login01 ~]$ chmod -rwxr-xr-x data_demo/writing_new/
[ese-zhaoan@login01 ~]$
```

1.10

```
[ese-zhaoan@login01 data_demo]$ history 10
  170  exit
  171  cd data_demo/writing/
  172  cd ..
  173  ls
  174  zip test.zip test
  175  zip writing_new.zip writing_new
  176  ls
  177  unzip writing_new.zip
  178  history
  179  history 10
[ese-zhaoan@login01 data_demo]$
```

2

```
(my_mpi) [ese-zhaoan@login02 pdb]$ for file in *.pdb
> do
> du -b $file
> done
1516    aldrin.pdb
306     ammonia.pdb
1444    ascorbic-acid.pdb
1030    benzaldehyde.pdb
1830    camphene.pdb
5049    cholesterol.pdb
1090    cinnamaldehyde.pdb
1694    citronellal.pdb
2452    codeine.pdb
1158    cubane.pdb
895     cyclobutane.pdb
1384    cyclohexanol.pdb
695     cyclopropane.pdb
622     ethane.pdb
690     ethanol.pdb
2396    ethylcyclohexane.pdb
765     glycol.pdb
4209    heme.pdb
1064    lactic-acid.pdb
2562    lactose.pdb
11193   lanoxin.pdb
3395    lsd.pdb
2562    maltose.pdb
2164    menthol.pdb
422     methane.pdb
490     methanol.pdb
1869    mint.pdb
2288    morphine.pdb
2123    mustard.pdb
1680    nerol.pdb
2729    norethindrone.pdb
1828    octane.pdb
1226    pentane.pdb
2287    piperine.pdb
```