

C2110 *UNIX and programming*

Lesson 11 / Module 1

PS / 2020 Distance form of teaching: Rev1

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Bash + AWK + Gnuplot

The data is in the directory:


`/home/kulhanek/Documents/C2110/Lesson11`

Exercise 1

1. The prod006.out file contains results from molecular dynamics. The task is to extract the dependence of the temperature of the simulated system on time from the file and save this data to the file temp.out which will contain exactly two columns. The first column will be the time and the second column will be the temperature.

```
.....  
NSTEP =          500    TIME (PS) =          0.500    TEMP (K) =      288.02    PRESS =          0.0  
Etot   =          942.6248    Ektot   =          151.0990    Eptot   =          791.5258  
BOND   =          51.3204    ANGLE  =          292.3619    DIHED   =          176.5980  
1-4 NB =          17.7099    1-4 EEL =          981.4071    VDWAALS =          -68.3301  
EELEC  =          -494.7423    EGB    =          -164.7991    RESTRAINT =          0.1822  
EAMBER (non-restraint) =          791.3436  
.....
```

time temperature



For analysis of rst.out file, use language awk.
Compare the solution with bash implementation.

2. Display the temperature profile over time in the form of a graph.

Exercise 2

1. From file prod006.out extract the dependence of total energy (Etot), kinetic energy (EKtot) and potential energy (EPtot) on time. Display the course of individual energies in gnuplot and save it to energy.png file. Verify that the sum of potential and kinetic energy equals total energy.

time
↓

```
.....  
NSTEP =          500    TIME (PS) =          0.500    TEMP (K) =    288.02    PRESS =          0.0  
Etot   =          942.6248    EKtot   =          151.0990    EPtot   =          791.5258  
BOND   =          51.3204    ANGLE  =          292.3619    DIHED   =          176.5980  
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EELEC  =          -494.7423    EGB    =          -164.7991    RESTRAINT =          0.1822  
EAMBER (non-restraint) =          791.3436  
.....
```

Exercise 3

1. Write script(s) that will print a series of numbers 3^n for n from 1 to N to data.txt file. (10 points). The number N is entered by the user as the first argument of the script (5 points). Entry treatment (5 points). View in gnuplot the number series saved in the data.txt file, use non-interactive display (10 points).

Example of assignment for exam.

Exercise 4

1. Draw an equilateral right triangle in the file, the outline of which will be from the characters "*" (5 points) and fill with "@" characters (10 points). The length of the triangle cathetus and the file name are entered by the user interactively after starting the script (5 points). Input treatment: The triangle must contain at least one "@" character (5 points). The script will not allow writing to an existing file (5 points).

Example of assignment for exam.

Exercise 5

1. Finds all files with extensions .hpp and .cpp in the specified directory and write their number in total and then separately for .hpp and .cpp files to standard output (10 points), then the total number of lines in all found files and then separately for .hpp and .cpp files (10 points). Save the report in the file "summary.txt" (5 points). Analysed directory is specified as the first argument of the script. Input treatment (5 points): The analyzed directory must exist. Test data can be found in the directory pmflib.

Example of assignment for exam.

Exercise 6

1. Write awk script, which extracts from a file with quantum-mechanical analysis of the molecular complex by SAPT0 method the components of interaction energy in kcal / mol in the section "SAPT Results" at the end of the file. Specifically, electrostatics, exchange, induction and dispersion energies. The last column will contain the total interaction energy (Total SAPT0). You can find the test data in the "sapt0" directory.
2. Write bash script which performs the above analysis for all files ending ".out" The first column will be the name of the analyzed complex (filename without ending ".out") and then individual components of the interaction energy. Save the result to the text file "results.txt". The data is in the "sapt0" directory.