Sample Output for Frenkel & Smit Case Study 4

The file below is the output file `out` generated by the input script `run` distributed with the original distribution of Frenkel and Smit's case studies. The output file contains a lot of information, not all of which is relevant for our purposes. Relevant information about the initial state of the system is highlighted in blue, and output information is highlighted in green. Look over this output file and make sure you understand what each highlighted section means. Some comments have been added in blue text to the highlighted sections (particularly the portions where the text of the output file is in error!!!).

```
--- temp 0.728
 ***************** MC_NPT ***************
  ******** test random numbers ***********
  i,ranf()             1  0.1271888239207311
  i,ranf()             2  0.7570476628140380
  i,ranf()             3  0.4756639577616939
  i,ranf()             4  0.1291914953129002
  i,ranf()             5  0.5637841812261476
 Initialisation on lattice:
       108 particles placed on a lattice
 Initial temperature     : 0.725
 Velocity centre of mass :
          x = 0.83E-16
          y = 0.29E-16
          z = -.21E-16
  Number of particles                          :       108
  Density                                      :     0.844
  Box length                                   :     5.039

  Initial Temperature                           :     0.725
    velocity centre of mass x-dir              :     0.000
    velocity centre of mass y-dir              :     0.000
    velocity centre of mass z-dir              :     0.000
  Time step                                     :     0.001
  Total simulation time                         :      0.50
  Equilibration                                 :      0.00
  Number of timesteps between two samples       :         1
  Number of timesteps between two samples g(r):          10
 Simulations with TRUNCATED AND SHIFTED potential:
 Potential truncated at                        :     2.500
 Energy shift                                  : -0.016317


 Total pot. energy in. conf.       :   -351.09710
 Total kinetic energy in. conf.    :    117.38202
 Total energy in. conf.            :   -116.33307
 Total virial initial configuration:   4319.14894
 ======>> Done   5.0000001E-02 out of   0.5000000      -233.5612402716311
```

The column below shows the total energy at the times indicated.

```
======>> Done    0.1000000      out of    0.5000000       -233.5661477610863
======>> Done    0.1500000      out of    0.5000000       -233.5693315527719
======>> Done    0.2000000      out of    0.5000000       -233.5696444020839
======>> Done    0.2500000      out of    0.5000000       -233.5702924912875
======>> Done    0.3000000      out of    0.5000000       -233.5745065276046
======>> Done    0.3500000      out of    0.5000000       -233.5722823463327
======>> Done    0.4000000      out of    0.5000000       -233.5727249418648
======>> Done    0.4500000      out of    0.5000000       -233.5741530822054
======>> Done    0.5000000      out of    0.5000000       -233.5705688344569
Energy and pressure calculated from g(r)
     Number of samples     :        50
     Average temperature   :     1.304
     Energy                :    -4.117
     Pressure              :     6.858

Shear viscosity:
 xy component :         0.000
 xz component :         0.000
 yz component :         0.000
 Average      :         0.000

   6.931664       0.0000000E+00
   20.66288       0.0000000E+00
   17.05785       0.0000000E+00
Total energy end of simulation    :   -233.21278
Total virial end of simulation    :   1596.03485
 ***** Calculate block averages ************
  number of averages             3
block data     1   0.668950  12.077576  -3.166155
block data     2   0.457262  12.971003  -2.848503
block data     3   0.558782  12.167592  -3.000839
block data     4   0.753736  10.802428  -3.293285
block data     5   0.898912   9.673625  -3.511009
block data     6   1.165247   7.922017  -3.910535
block data     7   1.432477   6.188818  -4.311404
block data     8   1.562258   5.248502  -4.506073
block data     9   1.608638   4.845416  -4.575642
block data    10   1.631843   4.638701  -4.610499
block data    11   1.585675   4.801063  -4.541204
block data    12   1.617232   4.585175  -4.588578
block data    13   1.553745   4.878790  -4.493333
block data    14   1.478296   5.268398  -4.380136
block data    15   1.506925   5.156448  -4.423117
block data    16   1.469086   5.424159  -4.366345
block data    17   1.423136   5.745111  -4.297406
block data    18   1.474664   5.514839  -4.374722
block data    19   1.541464   5.162076  -4.474919
block data    20   1.548569   5.137613  -4.485590
###### tot en        1.29684495          0.08620188
###### pot en        6.91046746          0.63288695
###### kin en       -4.10796470          0.12930768
  number of blocks          500
        0   0.0173   0.0005   0.1267   0.0040   0.0259   0.0008
        1   0.0244   0.0011   0.1794   0.0080   0.0366   0.0016
```

The three quantities below are static properties (and error estimates) from block averaging. NOTE THAT THE NAMES OF THE QUANTITIES LISTED IN THE FILE ARE WRONG!!

Temperature, T
Pressure, P
Potential Energy, U

2	0.0346	0.0022	0.2542	0.0161	0.0519	0.0033
3	0.0495	0.0045	0.3633	0.0329	0.0742	0.0067
4	0.0704	0.0091	0.5174	0.0668	0.1057	0.0136
5	0.1034	0.0195	0.7615	0.1439	0.1552	0.0293
6	0.1582	0.0457	1.1709	0.3380	0.2374	0.0685
7	0.2814	0.1407	2.0640	1.0320	0.4220	0.2110