Simulation Methods in Statistical Physics

(FK 8028)

Programming project report 4: Results and Statistics

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Introduction

The computed averages obtained for adjacent time steps are heavily correlated, thus the estimated errors of the averages would be underestimated. To counter this effect, one can implement the block averaging, which means dividing the data points into the blocks of the same length and averaging the data within each block. If the block length is sufficiently long, the data points become uncorrelated so one can perform a common statistical analysis on the block averages. The block averaging method is implemented in this part of the programming project to estimate errors of kinetic, potential, total energies and temperature of liquid argon system as well as Ar-Ar radial distribution function. Heat capacity of the simulated system is also estimated.

Method

80 ps MD simulation with 4 fs time step was performed for the system of 1000 Ar atoms at pressure ρ = 1374 kg/m^3 and starting temperature T = 95 K. For the first 300 steps of the simulation, velocities of every atom were rescaled to achieve the desired temperature, remaining trajectory was saved and used for analysis.

Heat capacity per atom in k_B units is estimated using the following equation:

$$\frac{C_V}{N} = \left(\frac{2}{3} - \frac{4 \cdot var(E_K)}{9NT^2}\right)^{-1}$$

(Derived from the book 'Compute Simulation of Liquids' by Allen and Tildesley)

Results

To perform the block averaging, one should calculate errors for some simple ensemble average (for example, kinetic energy), varying the block length. At first the errors will increase with increasing block length, but after certain block length the errors will converge to a value, corresponding to the set of independent data points.

On Figure 1 and 2, mean kinetic energy values with errors bars depending on the block time (block length multiplied by time step) are shown.

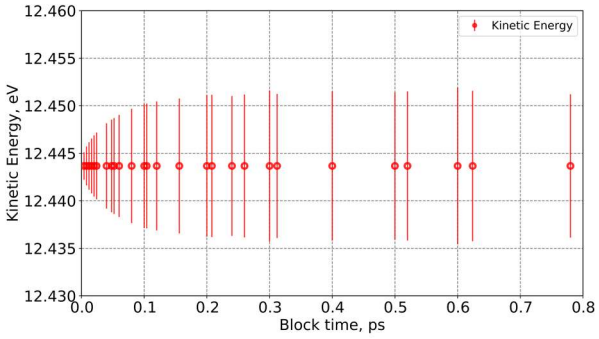

Figure 1 – Mean kinetic energy with error bars against the block time

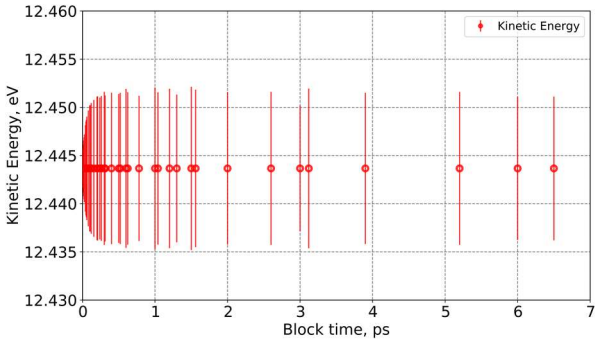

Figure 2 – Mean kinetic energy with error bars against the block time (extended block time scale)

On Figure 3 and 4, standard deviation and errors of the kinetic energy depending on the block time are shown.

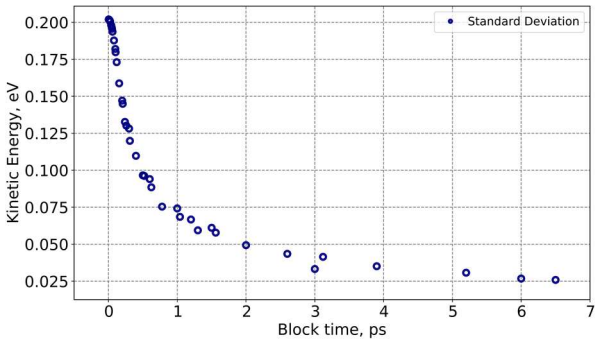

Figure 3 – Standard deviation of kinetic energy against the block time

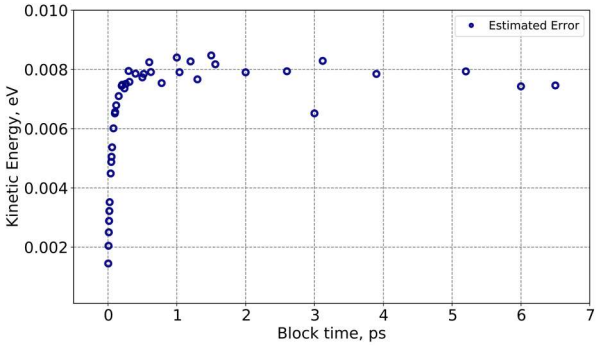

Figure 4 – Errors of kinetic energy against the block time

The error converges towards a stable value of approximately 0.008 eV. From the last figure it is possible to estimate the correlation time in the system which is around 1 ps of simulation time. This time corresponds to the block length of 250 steps – this number will be used for the future analysis.

On Table 1 computed averages with corresponding errors are presented.

Property	***Mean***	***Error***	***Unit***
E_k	12.4437	0.0084	eV
E_p	-59.8986	0.0084	eV
E_{Tot}	-47.45492113	$1.61 \cdot 10^{-6}$	eV
T	96.268	0.065	K
C_v	1.58	-	k_B

On Figures 5-7 computed radial distribution function and representation of the error bars are showed.

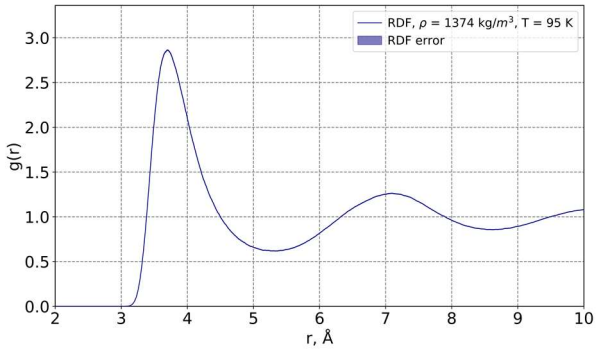

Figure 5 – Radial distribution function with error bars (global view, error bars are barely noticeable)

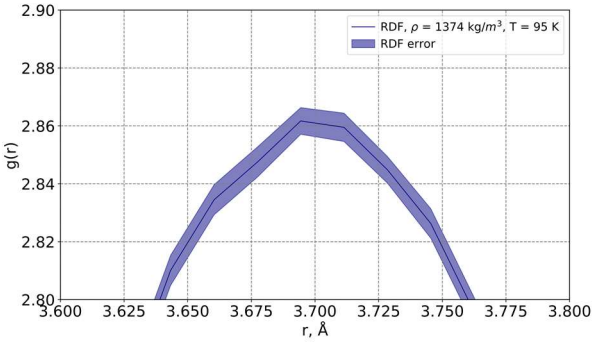

Figure 6 – Radial distribution function with error bars (first RDF peak)

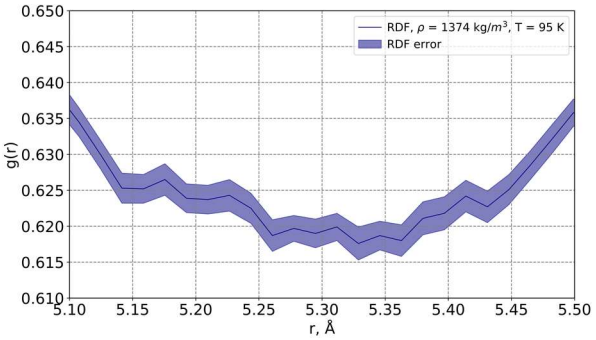

Figure 7 – Radial distribution function with error bars (first RDF minimum)

Obtained RDF errors are very small and are not higher than 0.0056 for the first RDF peak.

RDF peaks were compared with the data in Rahman paper in the previous report and it was shown that they match with the published data.

Conclusion

Block averaging is a very simple method that allows to estimate errors without explicit calculation of velocity autocorrelation function (which is relatively costly to compute). Even with the block averaging and removing correlation from the data set, obtained errors are generally much smaller, compared to the average values.