Exercise 2

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In reduced units, the potential, pressure, and their tail correction are as follows:

Potential

$$U(r)^* = \frac{e^{-r^*}}{r^{*2}}, \text{ for } r^* < {r_c}^*$$

Tail correction

$$U^{tail} = N2\pi\rho\int_{r_c}^{\infty} drr^2u(r)$$
$$U^{tail*} = N\pi e^{-{r_c}^*}$$

Pressure

$$P^* = \rho^* - \frac{1}{3V^*}\sum_{j<i}^{N-1}\sum_{i=1}^{N}\frac{\partial U^*}{\partial r^*} = \rho + \frac{1}{6N}\sum_{j<i}^{N-1}\sum_{i=1}^{N}(r^*+2)\frac{e^{-r^*}}{r^{*2}}$$

Tail correction

$$P^{tail} = \frac{2\pi}{3}\rho^2\int_{r_c}^{\infty} drr^3(-\frac{dU}{dr})$$
$$P^{tail*} = \frac{\pi}{6}(r^*+3)e^{-{r_c}^*}$$

1 Role of Δ

The average acceptance, average pressure and energy per particle with error for different Δ are shown in Table 1. As can be seen, when Δ increases, the average acceptance goes down, while the number of iterations to reach an equilibrium decreases. The average energy and pressure remain almost the same, which are the equilibrium values.

The average acceptance goes down because in the Monte Carlo simulation, all the particles are moved sequentially within a maximum displacement Δ. As Δ increases, the

energy difference between the old configuration and the new one increases. Therefore, there is a lower probability that such a move is accepted.

As for the decrease in the number of iterations, all the molecules are distributed with a random initial configuration. It takes time to thermalize and reach an equilibrium. (Figure 1) If Δ is large, the molecules move faster towards the equilibrium. (Figure 2)

The optimal value of Δ is between $L/2$ and L where the the acceptance is around 0.5 and the thermalization is fast. For the following computation, $L/2$ is taken as the optimal value of Δ.

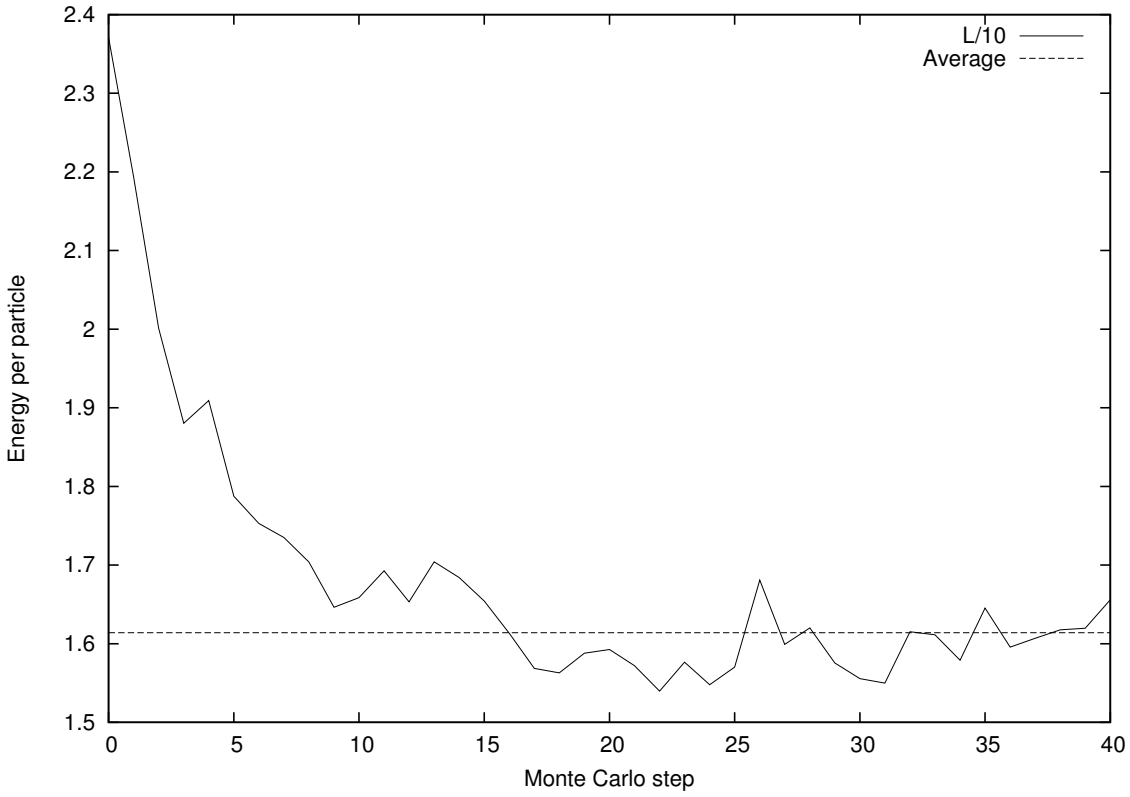

Figure 1: Energy Thermalization as the increase of Monte Carlo Steps for $\Delta = L/10$

2 Role of the cut-off

The average pressure and energy per particle with tail correction, P and E, and without tail correction, P^{nt} and E^{nt}, for different r_c are collected in Table 2.As the cut-off distance gets larger, P and E remain almost constant, while P^{nt} and E^{nt} increase. The difference

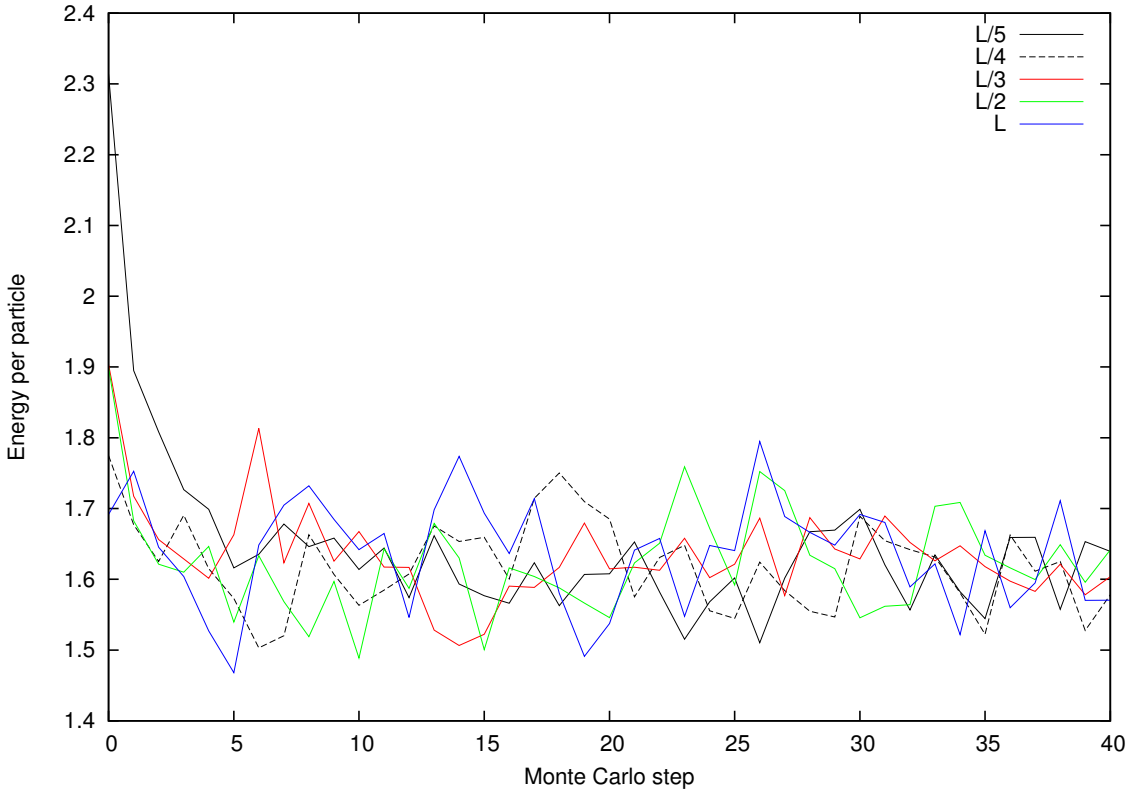

Figure 2: Energy Thermalization as the increase of Monte Carlo Steps for $\Delta = L/5, L/4, L/3, L/2, L$

Table 1: Average Acceptance, Average Pressure and Energy with Error for different Δ

Δ	Acceptance	P	σ_P	E	σ_E	Iterations
L/10	0.852438	1.481201	0.001373	1.614034	0.003086	16
L/5	0.720605	1.484285	0.000955	1.620900	0.002140	5
L/4	0.667223	1.483417	0.000824	1.618610	0.001889	4
L/3	0.591712	1.483086	0.000744	1.618221	0.001710	4
L/2	0.510158	1.483224	0.000525	1.618291	0.001216	3
L	0.439554	1.484713	0.000464	1.621889	0.001100	3

between with and without tail correction decays. This indicates that for a small cut-off distance, the tail correction perfectly makes up for the interaction with the molecules outside the range.

`Note:`

(1) For $r_c = 3L/4, 2L$, the cut-off distance is larger than $L/2$, the interaction with the image particles are taken into consideration.

(2) For $r_c = 2L$, the difference between with and without tail correction is so small that sometimes the randomness in initial configuration results in a larger value without tail correction than with tail correction, which is absurd.

Table 2: Average Pressure and Energy with and without tail corrections for different r_c

r_c	P	P^{nt}	ΔP	E	E^{nt}	ΔE
L/2	1.483332	1.209763	0.273569	1.618585	1.310095	0.30849
3L/4	1.483201	1.378177	0.105024	1.618544	1.520375	0.098169
2L	1.486700	1.483398	0.003302	1.624294	1.617679	0.006615

3 Size effects

The average pressure and energy per particle with tail correction, P and E, and without tail correction, P^{nt} and E^{nt}, for different N are shown in Table 3. The increase in the number of particles has a similar effect as the cut-off distance because when we fix the density of the system, the length of the box L, and therefore r_c, is determined by N. For a system with more molecules, the molecules could interact with a larger range of molecules.

Table 3: Average Pressure and Energy with and without tail corrections for different N

N	P	P^{nt}	ΔP	E	E^{nt}	ΔE
50	1.482670	1.209349	0.273321	1.617098	1.309108	0.307981
75	1.485613	1.276792	0.208821	1.623408	1.400749	0.222659
100	1.485790	1.318810	0.166980	1.623595	1.453968	0.183915
200	1.486215	1.398913	0.087302	1.623977	1.546434	0.077540