Worksheet X: NAME

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1 Running averages

In this section we had to calculate the running averages of the measured observables. The resulting plot can be seen below:
It can be observed that the observables fluctuate during the first time steps immensely and after some time they still fluctuate a bit, but their mean values become quite constant. This is due to the fact that first the system is equilibrating wherefore the observables fluctuate quite much, after this process the system is in equilibrium and therefore the observables stay constant. The time the system needs to be equilibrated is about $t_equi = 20$ time units. The mean values of the observables measured in one of our simulatios are:

Observable	Mean value
E_{tot}	1329.25
E_{pot}	-1671.12
E_{kin}	3000.38
T	2.00
P	0.6

2 Velocity rescaling

2.1 Derivation of the rescaling factor

It is:

$$\frac{k_b T}{2} = \frac{0.5 m v^2}{3N} \tag{1}$$

Which obviously leads to:

$$T_{mes} = \frac{m v_{mes}^2}{3N k_B}$$

$$T_{des} = \frac{m v_{des}^2}{3N k_B}$$

where T_{mes} is the measured and T_{des} is the desired temperature - analogous for the velocities. Calculating the factor $\frac{T_{mes}}{T_{des}}$ and solving for v_{des} leads to:

$$v_{des} = v_{mes} \sqrt{\frac{T_{des}}{T_{mes}}} \tag{2}$$

Therefore you have to multiply the measured velocities v_{mes} by the factor $\sqrt{\frac{T_{des}}{T_{mes}}}$ in order to get a correct velocity rescaling.

This velocity rescaling has been implemented in the python part due to the fact that it's a simple multiplication with a factor and nothing numerically problematic.