Project 1

FYS4460 - Disordered systems and percolation

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a)

I have used the following workflow to see how the velocity distribution evolves with time:

- LAMMPs generates an fcc structure, and saves a data file.
- A python script reads the data file, and replaces the velocities (which are zero) with uniformly distributed velocities in a specified range.
- LAMMPs runs a simulation from the resulting data file.
- A python script uses ovito to parse the simulation data, makes histograms for each saved frame and computes the correlation.

When calculating the histograms, I have made sure the same bins are used for all frames by first finding the maximum velocity attained by any atom during the simulation, and then using equally sized bins in the range $[-v_{\max}, v_{\max}]$. One histogram is computed for each direction, and then the average of these is taken.

The correlation is computed by normalising the histograms and taking the dot product with the histogram computed from the final frame. As the velocity distribution approaches the final distribution, the correlation should approach 1.

From figur 2 on the following page it is clear that the velocity distribution rapidly changes from a uniform to a gaussian shape. Figur 1 on the next page indicates that this happens exponentially, i.e.

$$C(t) = 1 - C_0 e^{-t/\tau},$$

where $C(t)$ is the correlation, C_0 is the initial correlation and τ is a time constant. If this is the case,

$$\ln(1 - C) = \ln\left(C_0 e^{-t/\tau}\right) = \ln(C_0) - t/\tau$$

so when plotted on a logarithmic scale, $1 - C(t)$ should be a linear function with slope $-1/\tau$.

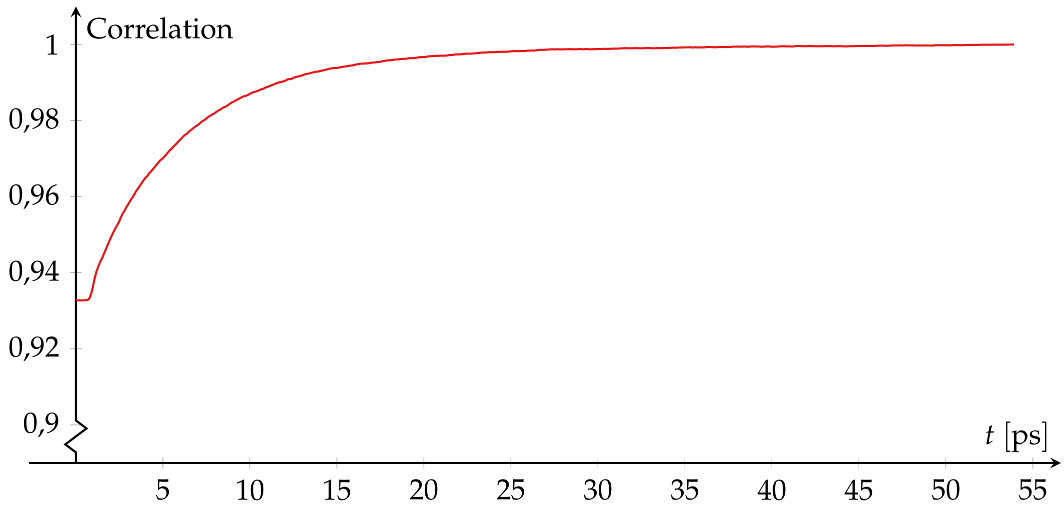

Figure 1: Correlation of the velocity distribution as a function of time.

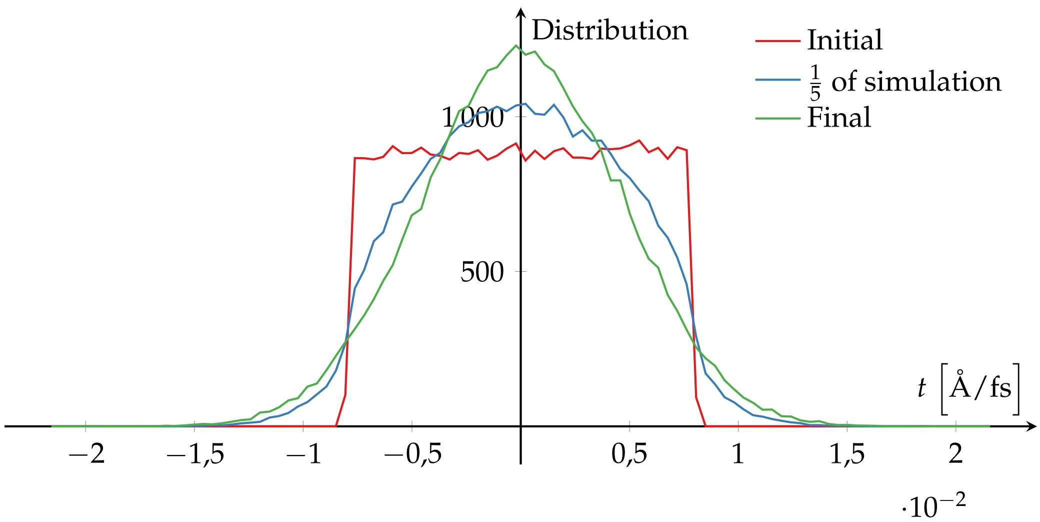

Figure 2: Distribution of the particle velocities in the initial and final configurations, as well as after one fifth of the simulation time.