Computational Physics Sommersemester 2025

Exercise Sheet 04

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Contents

1 Part a

In part a, we first included the walls like explained in the sheet. The implementation can be found in *force.py* and *update.py* in the functions `forceLJ_wall_z` and `VelocityVerlet_wall_z`. We implemented the force calculation of the wall in the same loop as the LJ force calculation, thus we had to add the force calculation for the particle with the highest index since the LJ force calculation only goes up to $n-1$ due to the particles not interacting with themselfes.

This resulted in the desired behavior where the particles were reflected by the wall while conserving pbcs in $x-$ and $y-$direction. A representative snapshot can be found in fig. 1.

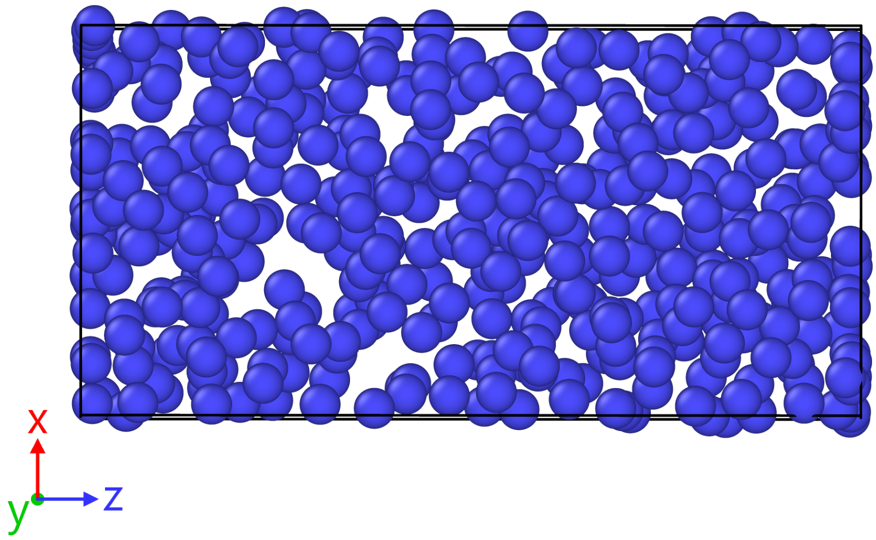
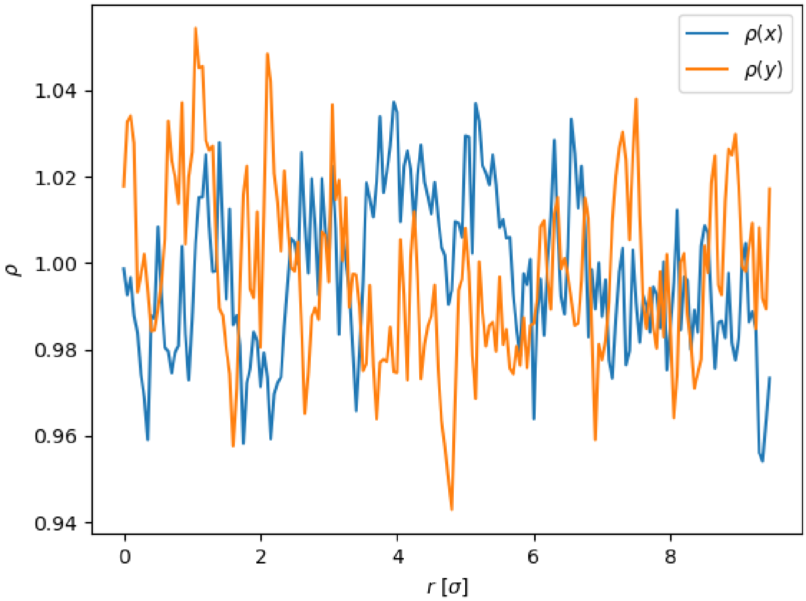


Figure 1: Snapshot of the last production timestep.

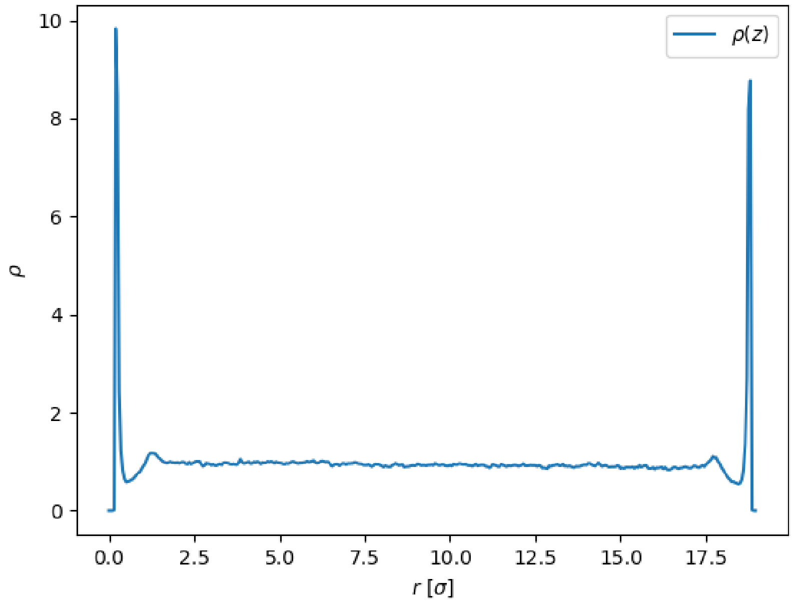
Then we calculated the particle densities in the respective directions and normalized to 1; the implementation can be found in *g_ r.py*. We ended up with the results displayed in fig. 2. We used the following formula to normalize the histogram:

$$n(b)_{\text{norm}} = \sum_{i}^{N/N_{gr}} \frac{n_i(b)}{N_{gr} N b_{max}} \tag{1}$$

where b is one bin and i is one histogram obtained by the analyzing steps and b_{max} the number of bins.



(a) $\rho(x, y)$



(b) $\rho(z)$

Figure 2: 1d–particle densities in the respective directions.

In fig. 2, we can clearly see that in the $x-$ and $y-$direction, the particles are distributed in an isotropic way like one would have suspected for this setup. However, a different profile appears for the $z-$direction with a vanishing ρ very close to the walls and a peak directly after, which can be attributed to the minimum in the potential of the wall.
The overall behavior fits to the shape discussed in the lecture.

We then calculated the mean force per particle on the walls, where we added

$$\langle F \rangle = \frac{1}{N_{\text{gr}} \cdot N_{\text{particles}}} \cdot \sum_{i,t} \text{sign}(r_i)(F_i(t)),$$

as implemented in *part_ a.py*. t describes the timestep while r_i is the distance of the particle to the wall according to the minimal image convention, otherwise the forces would be 0 in the mean due to the symmetry of the setup.

After dividing by the surface S, we ended up with a pressure of $0.280 \, \frac{\text{g}}{\text{mole}} \frac{\text{nm}}{\text{fs}^2} \cdot \frac{1}{\text{nm}^2}$. This means that the walls would be pushed apart by the particles if they weren't fixed.

2 Part b

In order to obtain the adsorption Γ defined as

$$\Gamma = \int_{z_{w,1}}^{(z_{w,1}+z_{w,2})/2} (\rho(z) - \rho_b) \, dz \tag{2}$$

we cut the array with all histograms taken every 10th step (N_{gr}) into 6 blocks and used all histograms in one block to calculate the density profile $\rho(z)$ to calculate Γ. We calculated ρ_b taking some values from the middle of the profile. With the standard deviation given by:

$$\text{Error}(\Gamma) = \sqrt{\frac{1}{N(N-1)} \sum_{i=1}^{N} (\Gamma_i - \langle \Gamma \rangle)^2} \tag{3}$$

block	**Value**
Adsorption 1	1.64
Adsorption 2	1.62
Adsorption 3	0.95
Adsorption 4	0.66
Adsorption 5	1.36
Adsorption 6	0.64
Statistical error Error(Γ)	0.19

Table 1: Adsorption values with statistical error

3 Part c

As told in the task, we simulated the fluid with $\epsilon_{\text{fluid}} = 0.25 k_B T_0$ and three different values for ϵ_{wall} as you can see in fig. 3. Here, one can see that a higher attraction of the wall results also in a higher probability to find particles close to the wall. But it is interesting that one can see a higher peak on the left side than on the right side in fig. 3. This can be attributed to unsufficient sampling, which also can be seen at the fact that for the smallest attraction, we observe to opposite asymmetry.
Furthermore, the position of the peak is almost the same for each ϵ. The density between the walls also does not depend on the attraction of the wall.

With a bit of imagination, one might also see this in the corresponding snapshots as seen in fig. 4.

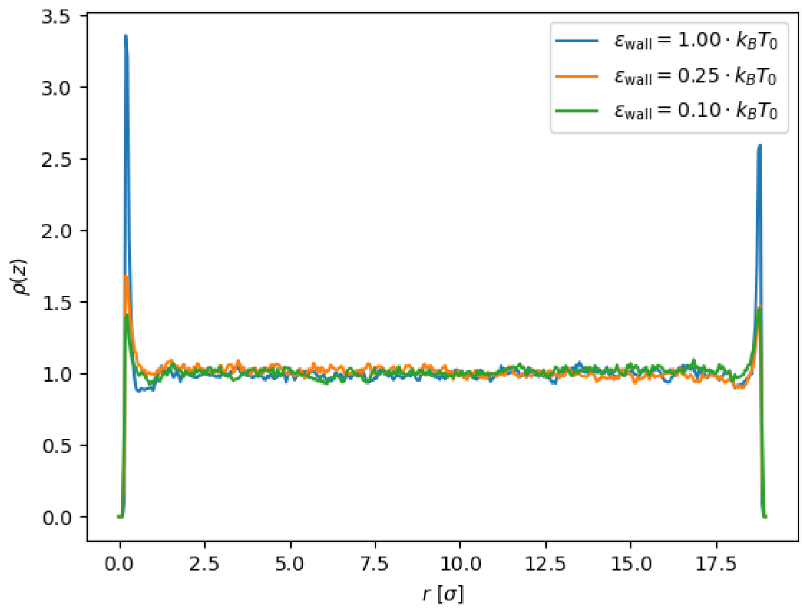
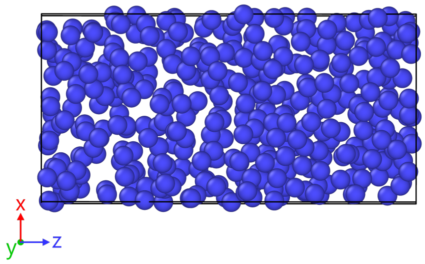
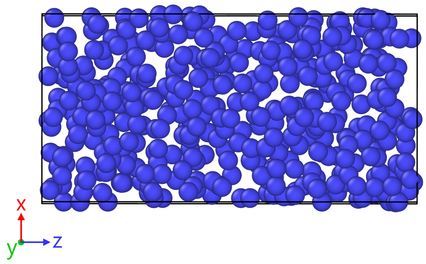


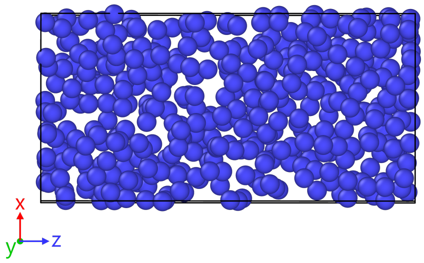
Figure 3: Comparison of different ϵ_{wall}



(a) $\epsilon = 0.10$



(b) $\epsilon = 0.25$

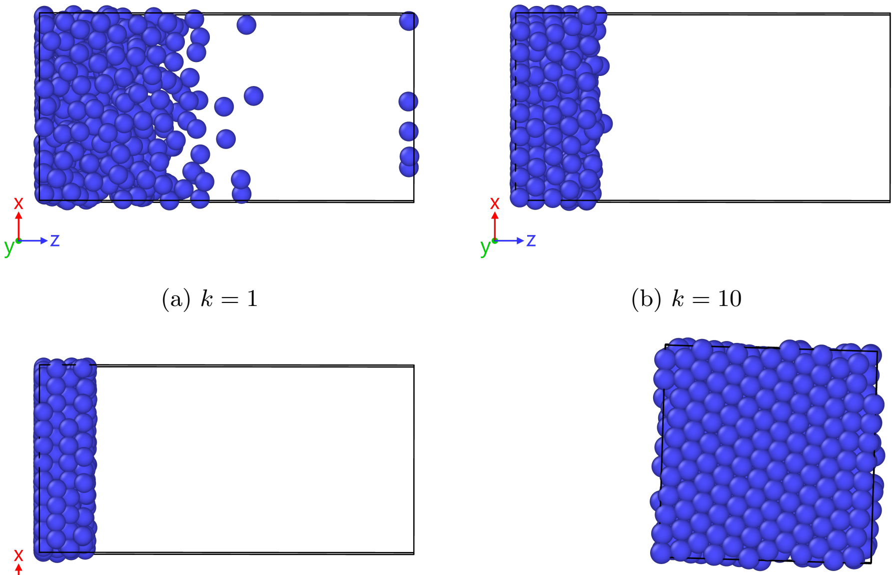


(c) $\epsilon = 1.00$

Figure 4: Ovito Snapshots of the last timestep.

4 Part d

In part d, we added an attractive external potential. As you can see in the pictures, a higher k results in a more dense structure. In fig. 6 one can see that the density profiles for each k.



(a) $k = 1$

(b) $k = 10$

(c) $k = 100$

(d) $k = 100$ View from the bottom

Figure 5: Ovito Snapshots of last timestep

Interestingly, one can see few particles sticking at the top of the box in the case of $k = 1$. Here the force of the wall is higher than the applied force. Almost like water drops hanging on a surface. If you look at $k = 100$ you can see that no particles are moving 'freely' anymore. All form a dense structure and form a lattice, as can be seen from the bottom perspective.

When plotting the density profile, this layering can be seen even more; at the same time, the exponential decay can be identified in fig. 6.

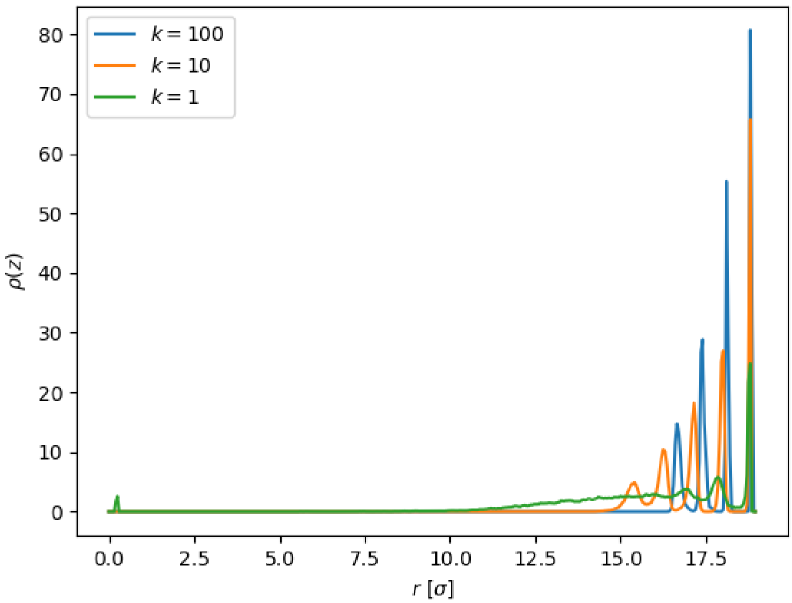


Figure 6: $\rho(z)$ density profiles for different k