Universität Freiburg – Institut für Physik
Applied Theoretical Physics
Prof. Dr. J. Dzubiella

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Exercise 4 for '*Computational Physics - Material Science*', SoSe 2021
Email: adnan.gulzar@physik.uni-freiburg.de, sebastien.groh@physik.uni-freiburg.de
Tutorials: Dr. Adnan Gulzar and Dr. Sebastien Groh

Please provide a well documented submission of your solution. Your submission should include

- A pdf file containing the solution to the questions with the corresponding equations that are implemented in your codes. Figures must contain axis titles with corresponding units and a caption.
- The source code should be commented, and the equations given in the pdf file have to be referenced in the source code.
- There is no need to provide the trajectory files.
- In case your code is not working properly, please provide a description of the debugging attempts you did.

Exercise 4.1: External Fields: Confined LJ Fluid Between Two Walls

Let us consider the 3D space divided in two regions. The region (half space) defined by $z < 0$ is occupied by a homogeneous solid (continuum), while an atom is located at $z = z_f > 0$. The total interaction energy between the solid and the atom, U_{wall}, is of the 9-3 LJ form (will be justified in the lecture):

$$U_{\text{wall}}(z_f) = \frac{3\sqrt{3}}{2}\epsilon_{\text{wall}} \left[\left(\frac{\sigma_{\text{wall}}}{z_f} \right)^9 - \left(\frac{\sigma_{\text{wall}}}{z_f} \right)^3 \right] ,$$

where σ_{wall} and ϵ_{wall} describe the characteristics of the wall-atom interaction. The interaction acts on the atoms within a cut-off distance, $z_{\text{max}} = 2.5\sigma_{\text{wall}}$, in the direction normal to the wall. Such an approach is commonly used to model the interactions between a structureless ('coarse-grained') solid wall and a liquid.

The objective of this exercise is to simulate a LJ fluid confined between **two** of those structureless walls in the microcanonical ensemble, as illustrated in Fig. 1. Use a LJ-fluid containing $N = 6 \times 6 \times 12$ atoms included in a simulation box of volume V with dimensions $L \times L \times 2L$ along the x, y, and z directions such that the number density is $\rho = N/V = 0.5\sigma^{-3}$. The walls, located at $z_{w,1}$ and $z_{w,2}$ (in distance $2L$), act on the LJ fluid along the direction normal to the walls, z, through $U_{\text{wall}}(z - z_{w,1})$ and $U_{\text{wall}}(z_{w,2} - z)$, respectively.

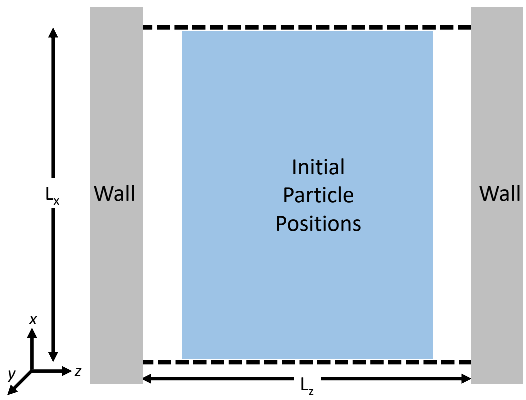

Abbildung 1: Schematic representation of a simulation box with two walls (gray), where the initial particle positions are constrained to the area in blue.

a) What boundary conditions would you have to apply to simulate the LJ fluid confined by two walls which we assume are 'infinitely' repeated in $x-y$ directions? Enrich the 3D MD implementation of Exercise sheet #3 with a function that calculates the solid-liquid interactions acting on the LJ fluid. Test your implementation with $\epsilon_{\text{fluid}} = \epsilon_{\text{wall}} = 0.5k_BT$, $\sigma_{\text{fluid}} = 5\sigma_{\text{wall}} = 2.55 \times 10^{-10}m$, and $T = 300K$. The equilibration and production runs of the confined fluid are performed during 2000 and 10000 steps, respectively. Provide a representative ovito-snapshot obtained at the end of the production run.

   The density profile, $\rho(z)$, as a function of the position along the direction normal to the walls, z, is defined as $\rho(z) =< \sum_i \delta(z_i - z) >$, where δ is the Dirac delta-function, and the sum index, i, runs over all the atoms. $< ... >$ is the average. Similarly, one can define the density profiles in the directions parallel to the walls, $\rho(x)$ and $\rho(y)$.

   Calculate and plot the density profiles along x, y, and z. Comment your results. Calculate and report the pressure on the two walls exerted by the fluid (the pressure is defined as $< \sum_i F_{w,i}(z) > /S_w$ where $F_{w,i}$ is the force exerted on the wall by the particle i on the the wall's surface with area S_w. The average $< .. >$ also includes the average over all particles. What would happen if the walls are not fixed but can freely move?

b) Perform similar simulations as in (a) but now with $\epsilon_{\text{fluid}} = 0.5k_BT$ and $\epsilon_{\text{wall}} = 0.1k_BT$ and $\epsilon_{\text{wall}} = 5k_BT$. Provide representative ovito-snapshot obtained during the production run for each value of ϵ_{wall}. Plot on the same plot the density profile, $\rho(z)$ versus z for the three values of ϵ_{wall}. Interpret your results.

c) Perform similar simulations as in (a), but now with applying an external constant force, $F^{app} = k\epsilon_{\text{fluid}}/\sigma_{\text{fluid}}$ with $k \in (1, 10, 100)$, on each atom of the LJ fluid along the z-direction. The equilibration and production runs are 10^4 time steps, respectively. Provide an ovito-snapshot at the end of each production run. Interpret your ovito-snapshot.

Numerical values of quantities to be used:

quantity	value (units)
k_B	1.38×10^{-23} (m^2 kg s^{-2} K^{-1}
ϵ_{fluid}	0.5 k_BT or text
σ_{fluid}	2.55×10^{-10} (m)
T	300 (K)
mass	105.52×10^{-27} (kg)
Δt	10^{-15} (s)