COMPUTATIONAL PHYSICS - EXERCISE SHEET 04
Lennard-Jones Fluid with Wall Interaction

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The following is the report for the Exercise Sheet 04. The goal of this exercise is to simulate a Lennard-Jones fluid confined between two structurless walls in the microcanonical ensemble. Along this report, python scripts were also handed in. Additional code can be found at the github repository given at the end of this page.

I. CODE IMPLEMENTATION

The new code implements the interaction between particles and two structurless walls positioned at $z = 0$ and $z = 2L$, given by the following 9-3 Lennard Jones potential:

$$U_{wall}(z_f) = \frac{3\sqrt{3}}{2}\epsilon_{wall}\left[\left(\frac{\sigma_{wall}}{z_f}\right)^9 - \left(\frac{\sigma_{wall}}{z_f}\right)^3\right] \tag{1}$$

where σ_{wall} and ϵ_{wall} describe the characteristics the the wall-atom interation. Additionally, as in the usual LJ interaction, a cutoff distance of $z = 2.5\sigma_{wall}$ is implemented.
The simulation consists of a volume V with dimension L x L x $2L$ and $N = 6$ x 6 x 12 particles. It also to be noted that given the presence of the walls, boundary conditions on the z axis are no longer necessary. Indeed the interaction between wall and particle keeps them bounded inside the volume; the same applies for the *minimum image convention* for calculating the distance between particles.

Furthermore the code computes the density profile ρ over a given axis, which describes how the particles are distributed in the volume, given by (for the z axis)

$$\rho(z) =< \sum_i \delta(z_i - z) > \tag{2}$$

Such profile is computed by doing a normalized histogram of given bin size (nbins = 50 for x-y, nbins = 100 for z), averaged for all the production iterations.

Lastly the pressure on the two walls is computed by averaging the forces from the wall-particle interactions and then dividing it by the surface area of the walls in the following way:

$$P =< \sum_i F_i(z) > /S \tag{3}$$

The pressure is provided for the lower ($z = 0$) and upper ($z = 2L$) walls.

II. TEST RUN

The first run is done with the usual parameters, namely:

- $\epsilon_{fluid} = \epsilon_{wall}$
- $\sigma_{fluid} = 5\sigma_{wall}$
- 2000 equilibration iterations
- 10000 equilibration iterations

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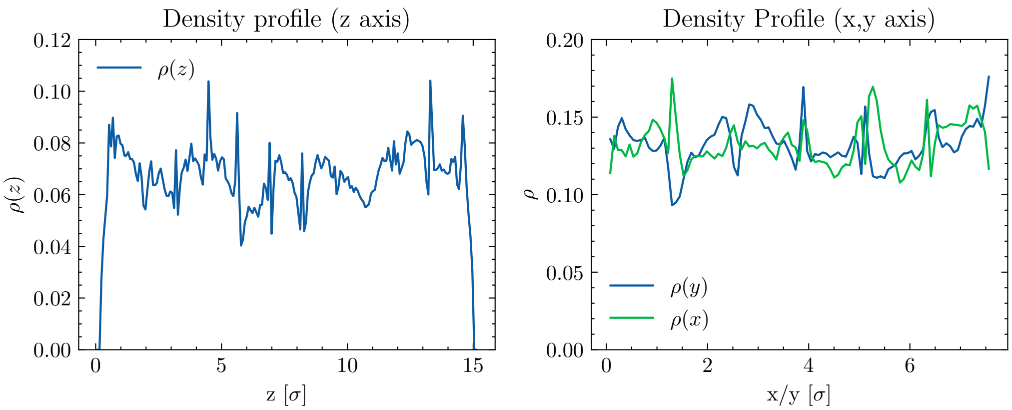

FIG. 1. The figures show the density profiles over the z axis (left) and x,y axis (right).

The following figure shows the density profiles.

Additionally the computed pressure are (note that the provided values are absolute in sign and reflect the outwards pressure on the walls):

- $P(z=0) = 0.122$ [reduced units]
- $P(z=2L) = 0.123$ [reduced units]

The similar values reflect the fact the interaction is symmetric and not dependent on the value of z but only on the distance from the walls. This will no longer be the case in the scenario of an external force. It is also interesting to note that if the walls were not fixed but able to move, the pressure from the particles would push them outwards, enlarging the volume of the box.

III. SIMULATING DIFFERENT VALUES OF ϵ_{wall}

The second part of the exercise consists in the simulation of the system using different values of ϵ_{wall}, namely:

- $\epsilon_{wall} = 0.2\epsilon_{fluid}$
- $\epsilon_{wall} = 10\epsilon_{fluid}$

A. Pressure

Since the parameter ϵ_{wall} represents the energy well of the potential, this is reflected in the density profile and in particular in the pressure on the walls. Indeed, a larger ϵ_{wall} corresponds to larger pressure. The following are the results for the lower pressure (where normal is the reference value of the test run)

- smaller ϵ: $P(z=0) = 0.092$ [reduced units]
- normal ϵ: $P(z=0) = 0.122$ [reduced units]
- larger ϵ: $P(z=0) = 0.240$ [reduced units]

and the following for the upper pressure:

- smaller ϵ: $P(z=2L) = 0.102$ [reduced units]
- normal ϵ: $P(z=2L) = 0.122$ [reduced units]
- larger ϵ: $P(z=2L) = 0.252$ [reduced units]

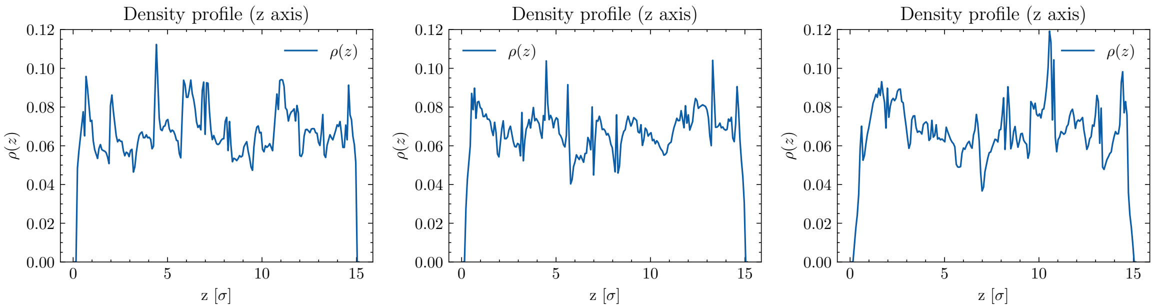

FIG. 2. The figure shows the density profiles $\rho(z)$ for different values of epsilon: smaller (left), reference (center), and larger (right).

B. Density profiles

IV. SIMULATING SYSTEM WITH EXTERNAL FORCE

The last part of the simulation consists in adding an external force of the following form

$$F^{app} = k\frac{\epsilon_{fluid}}{\sigma_{fluid}} \tag{4}$$

with $k \in \{1, 10, 100\}$, acting on the particles in the z direction.

A. Pressure

The way it was implemented lead to an accumulation of particles on the lower wall, resulting therefore in an high pressure on that specific wall. On the other hand the other wall did not feel any significant pressure. The results can be understood quite intuitively. The following are the values of the pressure on the lower wall

- $k = 1$: $P(z = 0) = 0.33$ [reduced units]
- $k = 10$: $P(z = 0) = 1.02$ [reduced units]
- $k = 100$: $P(z = 0) = 2.62$[reduced units]

B. Density profiles

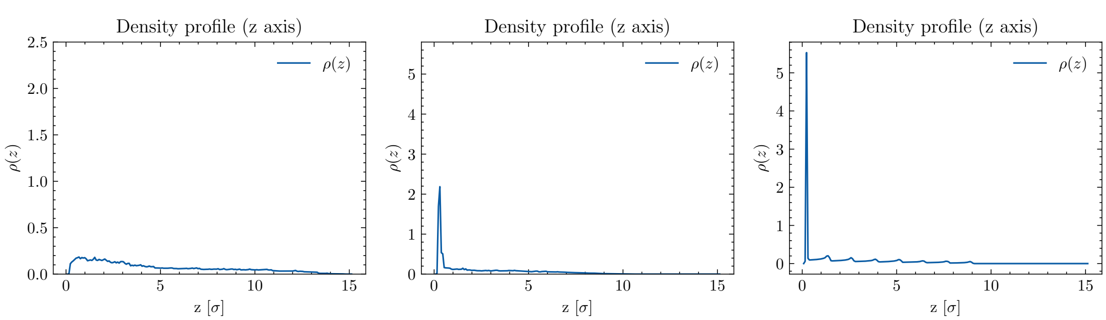

FIG. 3. The figure shows the density profiles $\rho(z)$ for different values of k: $k = 1$ (left), $k = 10$ (center), and $k = 100$ (right). Note that the ρ range for k=1 is halved compared to the others.

V. OVITO SNAPSHOTS

The following are some of the ovito snapshots from the various simulation. Note that some have been omitted due to the fact that they did not show any significative results.

A. Test Run

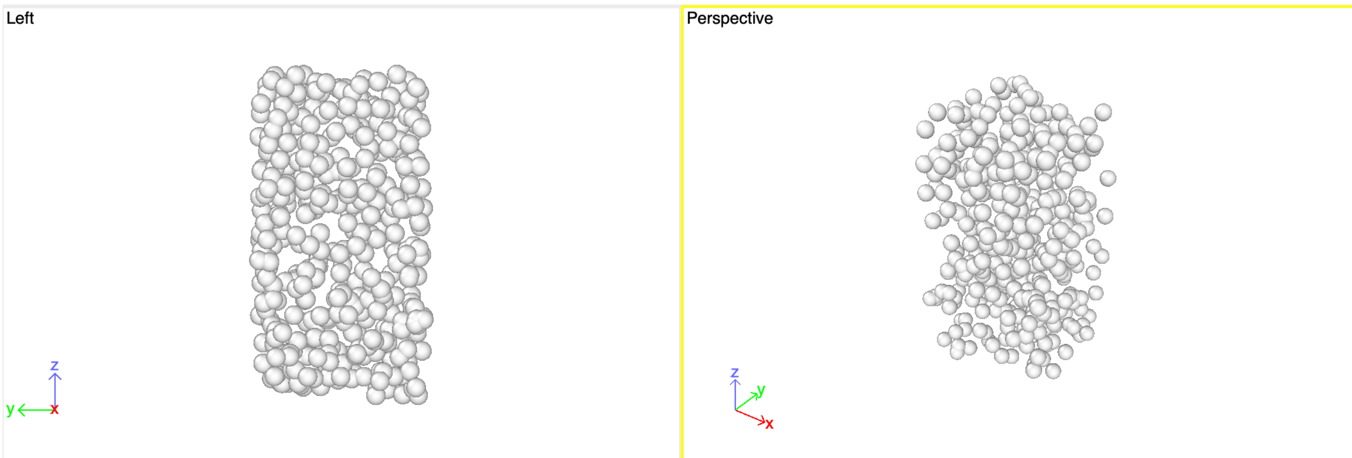

FIG. 4. The figure shows an Ovito snapshot after the production run of the test run

B. Large epsilon

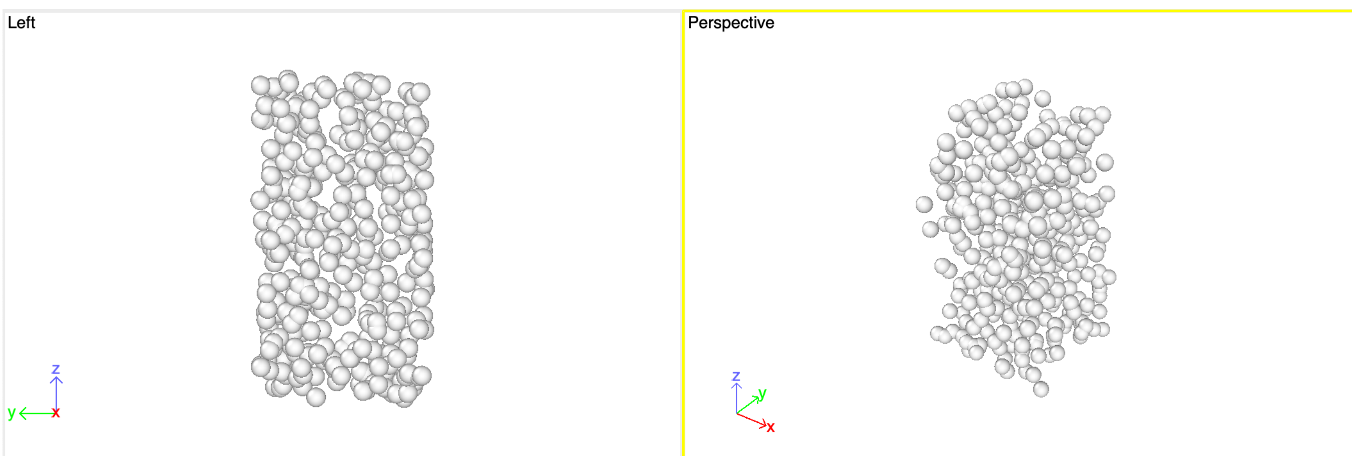

FIG. 5. The figure shows an Ovito snapshot of a system with $\epsilon_{wall} = 10\epsilon_{fluid}$.

C. External force k=10

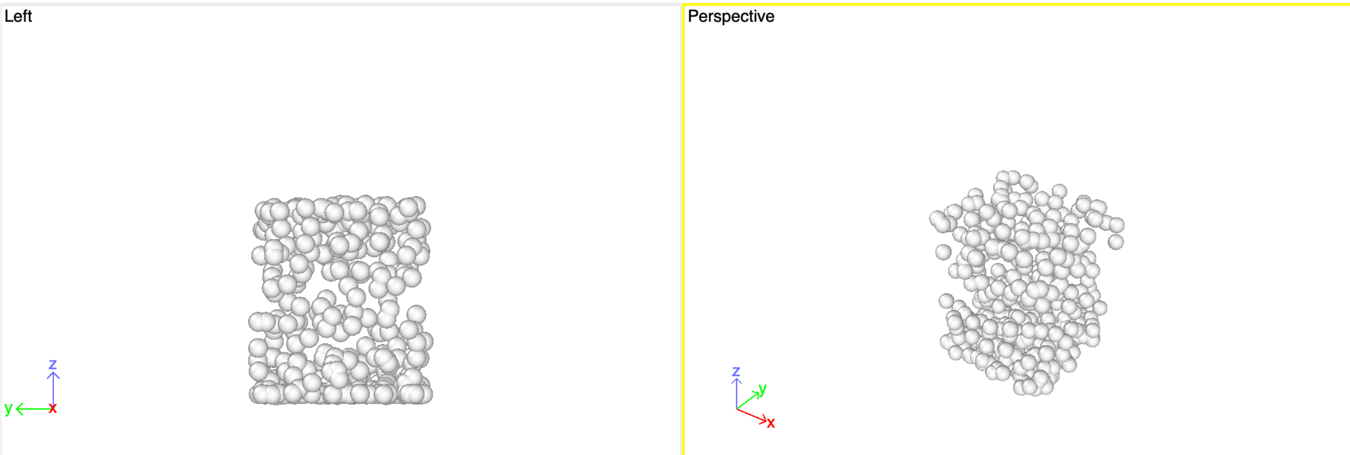

FIG. 6. The figure shows an Ovito snapshot for a system subject to external force with $k = 10$

D. External force k=100

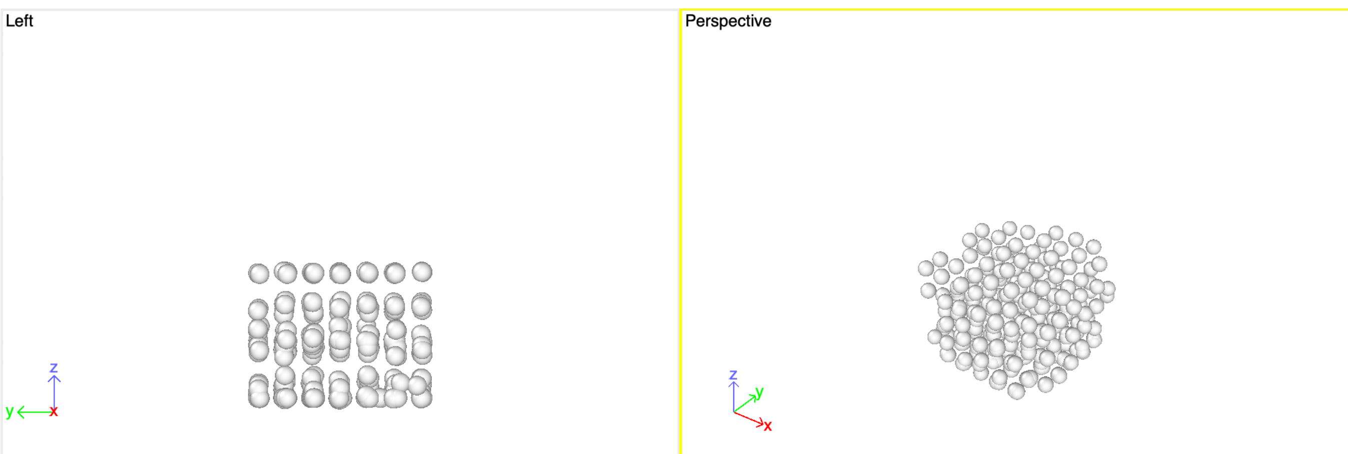

FIG. 7. The figure shows an Ovito snapshot for a system subject to external force with $k = 100$