Detailed investigation on the effect of wall spring stiffness on velocity profile in molecular dynamics simulation

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Abstract. In this paper, motion of 576 monatomic argon molecules is studied in a channel with two 2-layered wall molecules. The effect of wall spring stiffness (K) on maximum value of velocity profile is investigated in the channel. It was observed that for $K<500\, \text{ergs/} \cdot \text{mol}$, there is a decrease in the maximum value of velocity profile with an increase in $K$. This observation has been already reported by Sofos et al. To investigate a wider range of spring stiffness, in this paper the value of $K$ was increased to more than $500\, \text{ergs/} \cdot \text{mol}$. In this range of wall spring stiffness the behavior of maximum value of velocity profile changed; it increased with an increase in $K$. In a separate simulation the external force applied to the molecules was also increased and the same non-monotonic behavior of maximum value of velocity was observed. To clarify the reason of this behavior, the concepts of original and effective wall are introduced and through several test it is inferred that the mentioned concepts are not successful to demonstrate the reason of such behavior. It is suggested to obtain non-dimensional parameters governing the simulation in order to investigate the effect of every involved parameter on such a behavior. It is finally concluded that while wall spring stiffness affects the maximum velocity magnitude within the flow, the interaction of the two has not been clearly shown yet. The behavior of the maximum velocity is non-monotonic with the change of $K$. This is why no specific criterion has been reported for suitable value of wall spring stiffness in molecular dynamics simulation.

1. Introduction
The progress of human science has resulted in smaller devices and systems like nanotubes and Micro Electro Mechanical Systems (MEMS). Microscopic fluid flow like heat transfer in a thin film of solids or flow in a nano-channel has consequently arisen. Since conventional fluid mechanics fails to predict the flow characteristics in micro-nano scales [1], molecular dynamics simulation (MD) is used. MD simulation calculates the molecules' velocity and position in each time step and the flow characteristics like mean velocity, density, pressure and temperature is obtained using different methods of sampling[2].

In molecular dynamics one has to consider suitable boundary conditions as well as a proper model for a successful simulation. Wall boundary condition is one of the most important BCs which describes the molecules' behavior at a solid boundary. Needless to say, it is not possible to use no-slip boundary condition in MD simulation since the reflection of molecules after collision with the wall should be
calculated precisely based on molecular dynamics formulations and the modeling of wall molecules which is very important. Note that modeling of wall molecules could affect the fluid behavior both near the wall and far from it.

In 1977 Abraham used a function to introduce a continuous molecular wall [3]. He also modeled a molecular wall with separate solid molecules. Later in 1989 Joel Kuplik studied fluid flow at solid surfaces with use of MD simulation [4]. He used fixed molecules to model the molecular wall.

One of the most efficient methods for molecular wall modeling is to attach each molecule to its place with a spring. In this way the molecules will be forced back to their initial place when they are moved. Many simulations have utilized springs, whether linear or non-linear, in their molecular wall [1,6-9]. Although a wide range of spring stiffness (57-6000e$\sigma^{-2}$) has been used in different simulations yet there is not a specific criterion available for choosing proper spring stiffness. It is only assumed that spring stiffness should be high enough to prevent the fluid molecules from passing through the wall.

In this paper an investigation on spring stiffness is done to emphasize that the choice of spring stiffness is important in molecular dynamics simulation since different values of spring stiffness will result in different values of maximum velocity in a channel. However no method has been reported for choosing proper spring stiffness. The intention of authors has been to report some observations concerning the effect of wall spring stiffness on maximum velocity and channel’s effective width.

2. Molecular modeling and Solution Procedure

This paper presents the simulation of 576 liquid argon molecules ($\rho^* = 0.642 \sigma^{-3}$) which are conducted in a 36.15 Å channel. Although, the simulation carried out in this paper is for a liquid, the same procedure is applicable to gases.

The Knudsen number of the flow is 0.04 and the pressure is 50 Mpa. The velocity direction of each molecule is determined using Maxwell-Boltzmann distribution function. The interaction between molecules is described by Lennard-Jones 12-6 potential equation:

$$U_{ij} = 4\varepsilon \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^6$$

(1)

Where $U_{ij}$ is the potential energy, $r_{ij}$ is the distance between two interacting molecules $i$ and $j$, and $\sigma$ and $\varepsilon$ are the distance characteristic length and energy scale, respectively. The intermolecular forces are then calculated from equation 1 through the following relation:

$$F_{ij} = -\frac{dU_{ij}}{dr_{ij}}$$

(2)

And finally the motion of the molecules is determined by Newton’s second law through the Verlet’s integrating scheme [10].

As mentioned before, two 2-layered walls are located at Y-constant positions. In the other directions periodic boundary conditions are applied. Each wall molecule is attached to its place with a linear spring to ensure wall solidity. The spring will consequently exert a force of $F = -K\Delta r$ to every molecule that moves away a distance equal to $\Delta r$; in this equation $K$ is the spring stiffness. Figure 1 shows the schematic of initial placement of fluid and wall molecules.
Wall temperature is kept constant using thermostat. In fact at each time step velocity of wall molecules are rescaled to ensure constant wall temperature. An external force is constantly applied to the fluid molecules in order to develop flow in the channel. It should be noted that all of the initial conditions of the simulation such as temperature, number of molecules, spring stiffness, number of wall layers and external force magnitude are chosen similar to a simulation performed by Sofos et al [9] in order to validate the simulation of this paper. The detailed specifications of the simulation carried out in this paper are presented in table 1.

**Table 1.** Specification of the system under examination.

| Specification                      | Details                                    |
|-----------------------------------|-------------------------------------------|
| Dimension (Angstrom)              | 36.15×36.15×36.15                          |
| Wall molecules                    | 288 argon molecules                        |
| Fluid molecules                   | 576 argon molecules                        |
| Spring stiffness (εσ²)             | Different values                           |
| External force (pN)               | 0.18 and 1                                 |
| Thermostat (k)                    | Fixed on 120                               |
| Number of bins                    | 15                                         |
| Time step (s)                     | 10⁻¹⁴                                      |
| Boundary Conditions               | Periodic in X and Z directions             |
|                                   | Wall BC in Y direction                     |
3. Results and discussion

Having done several simulations with different values of spring stiffness, 3 major observations could be reported as below:

1. The maximum value of the velocity profile is plotted against spring stiffness. To manage this, the domain of flow is divided into 15 bins and the velocity profile is obtained by averaging the magnitude of molecules’ velocity in every bin using SMC method of averaging [2]. The result is shown in figure 2. Velocity profile is a proper variable to be observed with the change of spring stiffness since it well describes the flow throughout the domain and its convergence is relatively rapid.

Figure 2 shows that as wall spring stiffness (k) increases the value of maximum velocity in the channel decreases for K<500 $\varepsilon\sigma^{-2}$. This behavior of maximum velocity has been already reported by Sofos et al [9]. Note that all conditions of the present simulations including initial conditions, boundary conditions, wall molecule arrangement and its spring stiffness, number of molecules, channel width, and magnitude of external force are the same as those set by Sofos et al. For K>500 $\varepsilon\sigma^{-2}$ for which the simulation is not conducted by Ref. 9, calculations performed in the present study shows interestingly that the maximum velocity increases with the increase of K.

![Figure 2. Maximum velocity of channel vs. spring stiffness for $F_{ext} = 0.18$ pN](image)

Since the spring stiffness affects maximum value of the velocity profile, it can be inferred that for a channel with dimensions mentioned in Table 1, spring stiffness affects the flow even far from the walls. That's why the spring stiffness value has to be carefully chosen for such a channel.

2. In order to investigate the effect of the external force on the above issue external force is changed from 0.18pN to 1pN, in the above test case. Variation maximum velocity versus spring stiffness is plotted in Figure 3 for $F_{ext} = 1$ pN.
In this figure, after a small decrease in the maximum velocity for $K < 600 \varepsilon \sigma^{-2}$, it starts to increase up to about $K = 4000 \varepsilon \sigma^{-2}$, and then it again decreases. From these observations one can conclude that the maximum velocity do not obey a monotonic behavior.

3. Different scenarios were considered to clarify the reason of such behavior. Although we were not successful in this regard, one of the scenarios worth to be mentioned in this paper.

If the original width of channel is defined as the distance between the two walls at the beginning of the simulation, then an effective width of channel can be defined as the average distance between the displaced molecules of walls at the two sides of the channel, as shown in figure 4.

To explain the behavior of maximum velocity with spring stiffness we may assume that as the value of spring stiffness increases the oscillations of wall molecules are limited. This will result in a wider effective channel width and therefore a higher maximum velocity, as mentioned in [9] as well. Therefore maximum velocity should vary directly by spring stiffness.

**Figure 3.** Maximum velocity of channel vs. spring stiffness for $F_{ext} = 1 \text{pN}$
Several simulations have been carried out for different values of spring stiffness having external force of 0.18 pN to verify the above theory. Since the effective width of channel is a function of molecular behavior of simulation, its value should be time-averaged. For this purpose we have used SMC method of averaging. The results of the simulations are shown in table 2 and figure 5.

Table 2. Channel's effective width with change of spring stiffness.

| spring stiffness εσ⁻² | effective channel width (m) |
|-----------------------|----------------------------|
| 10                    | 2.964830E-09               |
| 30                    | 2.955200E-09               |
| 50                    | 2.956044E-09               |
| 70                    | 2.959049E-09               |
| 100                   | 2.963865E-09               |
| 150                   | 2.970468E-09               |
| 300                   | 2.984373E-09               |
| 500                   | 2.994998E-09               |
| 700                   | 3.001693E-09               |
| 1000                  | 3.008557E-09               |
| Standard deviation    | 1.889943E-11               |

Figure 5. Different effective channel width with change of spring stiffness.

Except for the first part of the figure 5, the rest of it can be explained based on the above-mentioned theory. Having compared figures 5 and 2 with each other, it can be seen that the trend of results are the same. However the turning points in these figures are not that close to each other. Although we put lots of efforts to offer better explanation for the behavior of maximum velocity with spring stiffness, it seems that we were not successful.
4. Conclusions and suggestions
Since the spring stiffness is able to affect the flow even far from the walls, suitable spring stiffness should be used for molecular dynamics simulations otherwise inaccurate results may be obtained. It is noticed that the behavior of maximum velocity magnitude is non-monotonic when the spring stiffness is changed for the both external forces applied in this paper. It first decreases and after specific spring stiffness it increases. The idea of original and effective width has been proposed to clarify the reason of such behavior; however it was not successful.

It is suggested that the tests done on the effective width be repeated with different external force magnitudes. To investigate all of the parameters affecting the velocity profile, it is proposed that the dimensionless parameters of this molecular dynamics simulation are obtained. In this way it is possible to study the reason of maximum velocity behavior considering all of the dominant parameters including spring stiffness, external force, channel width and etc.
5. References

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