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 $K<500\ \varepsilon\sigma^{-2}$, 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 $500\ \varepsilon\sigma^{-2}$. 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.