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# Smart Wall Model for Molecular Dynamics Simulations of Nanoscale Gas Flows

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**Abstract.** Three-dimensional molecular dynamics (MD) simulations of gas flows confined within nano-scale channels are investigated by introduction of a smart wall model that drastically reduces the memory requirements of MD simulations for gas flows. The smart wall molecular dynamics (SWMD) represents three-dimensional FCC walls using only 74 wall molecules. This structure is kept in the memory and utilized for each gas molecule surface collision. Linear Couette flow of argon at Knudsen number 10 is investigated using the SWMD utilizing Lennard-Jones potential interactions. Effects of the domain size on the periodicity boundary conditions are investigated using three-dimensional simulations. Domain sizes that are one mean-free-path long in the periodic dimensions are sufficient to obtain domain-size independent MD solutions of nano-scale confined gas flows. Comparisons between the two- and three-dimensional simulations show the inadequacy of two-dimensional MD results. Three-dimensional SWMD simulations have shown significant deviations of the velocity profile and gas density from the kinetic theory based predictions within the force penetration region of the walls.

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**Key words**: Rarefied gas flows, kinetic theory, surface effects.

## 1 Introduction

Gas flows in micron and nano-scale domains are frequently encountered in the components of micro electromechanical systems, microfluidic devices, and in computer hard drives. Especially for the hard-drive systems, distance between the head and media is on the order of tens of nanometers. Gas flow in such small scales cannot be described

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using the continuum hypothesis, and the Knudsen number, $Kn$, (ratio of the gas mean free path, $\lambda$, to the characteristic flow dimension, $H$) emerges as a measure of the degree of rarefaction. Depending on the local Knudsen number, the flow is considered to be in the continuum ($Kn \leq 0.001$), slip ($0.001 \leq Kn \leq 0.1$), transition ($0.1 \leq Kn \leq 10$), and free-molecular ($Kn > 10$) flow regimes [1]. Such characterizations assume "dynamic similarity" between the gas flows in low pressure environments (i.e., large $\lambda$) and small scale domains, which is valid for as long as one can neglect the surface force interactions between gas and wall molecules.

Rarefaction effects alone bring many challenges to the formulation of relevant constitutive laws and boundary conditions for high-order continuum models (in $Kn$). As a result, gas transport in small scales is often investigated using kinetic theory based on the Boltzmann equation. Analytical and numerical solutions of the Boltzmann equation are usually challenging due to the complexity induced by the collision integral terms and the multi-dimensionality of the equation. In addition, gas/wall interactions are often described using simple rules, such as the diffuse and specular reflection. More complex gas/surface interaction models, based on the Maxwell's scattering kernel [1] or Cercignani-Lampis model also exist [2]. Boltzmann equation can yield analytical solutions in the free molecular flow regime, where the intermolecular collisions can be neglected. Alternatively, one can utilize the Direct Simulation Monte Carlo (DSMC) method of Bird [3] to simulate flows in the slip, transition and free-molecular flow regimes. The DSMC could also include the gas/surface interaction models based on the aforementioned scattering kernels. Based on these theoretical and algorithmic developments there has been a vast number of investigations of gas flows in the late transition and free molecular flow regimes ($Kn \geq 5$) [4–14]. Unfortunately many of these studies assume "dynamic similarity" and neglect the gas/surface force interaction effects, which can be significant in nano-channel flows. For example, flow of argon (electrically neutral and monatomic) in $H$=6.48$nm$ height channel under standard conditions ($\lambda_{\text{argon}}$=64$nm$) results in $Kn$=10, which is in the free molecular flow regime. However, the van der Waals force interaction length-scale between an electrically neutral surface and argon molecule is approximately $1nm$ (about three molecular diameters, $3\sigma$). It is obvious that such force interactions would be effective within $1/3^{\text{rd}}$ of the channel, despite the free molecular flow regime predicted by the kinetic theory. Therefore, one must understand and evaluate the influence of this near-wall force field on the nano-scale confined flow, and characterize deviations from the kinetic theory predictions.

Molecular Dynamics (MD) may be utilized to characterize the gas/wall interactions. Literature on MD simulations of rarefied gas flows is rather limited. In a series of studies Cieplak *et al* investigated gas flows in nano-channels using three-dimensional MD simulations [15–18]. Particularly, [15] presents Poiseuille flow for $Kn = 0.03$, 0.12, and 5.52 in a nano-channel with $12.75\sigma$ in height, by assigning periodic boundary conditions along the channel length and width of $13.6\sigma$ and $5.1\sigma$, respectively. These simulations utilized purely repulsive and attractive wall models, and have demonstrated density accumulation effects near the boundaries, results of which have been quantified in [16].

Furthermore, differences in the velocity profiles from the predictions of continuum hydrodynamics are shown. In [17], the boundary conditions at the fluid/solid interface is presented for monatomic and chain molecules. Density immediately next to the surface for both kinds of fluids is shown to be largely independent of the bulk density for different $Kn$ values, driven by the attractive walls with large gas/wall interaction strength. The effect of patterned surface on both chain and simple fluid cases are presented in [18]. MD simulations of gas flows are computationally expensive due to the following reasons: First, gas flows evolve through intermolecular collisions characterized by the mean free path. Despite the large $Kn$ value induced by the nano-scale confinement, computational domain in the lateral and axial flow directions must be extended to a distance on the order of $\lambda$ to allow intermolecular collisions in these directions. This requirement results in simulation volumes on the order of $\lambda^3/Kn$ that contain a large number of gas molecules ($N\times\lambda^3/Kn$, $N$ being the number density). Second, the MD simulations must be executed for time-scales on the order of several intermolecular collision times to result in a state amenable for time or ensemble averaging. The third issue is the excessively large number of wall molecules required to atomistically model the surfaces, which induces extensive memory requirements.

The *objectives* of this paper include the development of a "Smart Wall" model that significantly reduces the memory requirements for MD simulations of gas flows (Smart-Wall-MD: SWMD). Using this model, we address the differences in two- and three-dimensional MD simulations, as well as the relevance of domain size and the effects of periodicity in MD simulations. Our computational model utilizes the 6-12 Lennard-Jones potentials for intermolecular interactions between the argon molecules, as well as argon and wall molecules. The new computational model enables MD simulations of linear Couette Flow in nano-channels with realistic surface force-field effects, and enables investigations of deviations from the kinetic theory based solutions.

This paper is organized as follows: In Section 2, we describe the SWMD algorithm along with the differences of the wall force field in two- and three-dimensions. We also summarize the parameters and methods utilized in the MD algorithm. In Section 3, we present the velocity and density profiles obtained using two-dimensional MD simulations. Section 4 includes discussions of the domain size effects on the periodicity boundary conditions, as well as the velocity and density profiles obtained in three-dimensional simulations. Finally, we present the conclusions of our study.

## 2 Theoretical background and model description

### Smart wall model

MD simulations of gas flows often require large computational domains, since gas flows evolve through intermolecular and molecule/surface collisions. Without loosing generality, we will examine channel flow at a given $Kn$ value. Depending on the base pressure and temperature one can find the number density of gas molecules ($N$) using the ideal

Table 1: Comparison of the number of molecules used in SWMD and typical MD simulations.

| $H=3.24nm, \lambda=32.4nm$ | Regular rarefied gas MD | | SWMD | |
|---|---|---|---|---|
| W × L | $N_{wall}$ | $N_{gas}$ | $N_{wall}$ | $N_{gas}$ |
| $\lambda\times\lambda$ | 36,603 | 200 | 74 | 177 |
| $3\lambda\times3\lambda$ | 325,803 | 1,800 | 74 | 1,593 |
| $5\lambda\times5\lambda$ | 903,003 | 4,900 | 74 | 4,425 |

gas law, and can also calculate the mean free path, $\lambda$ [1]. The simulation domain needs to encompass the channel height ($H$) in the transverse direction, and should be large enough to allow intermolecular collisions in the lateral and axial directions. For this reason dimensions of the simulation domain should extend at least one mean-free path in the lateral and axial directions. This requires a computational volume of $\lambda^3/Kn$ with a total number of gas molecules equal to $N\lambda^3/Kn$. For example, simulation of argon gas at $T=298K$ and $P=202kPa$ ( $\lambda_{\text{argon}}=32.4nm$) in $3.24nm$ height channel ($Kn=10$) with in a $\lambda\times L\times\lambda$ domain requires simulation of only 177 gas atoms (Table 1). However, these gas molecules interact with walls that cover an area of $2\times\lambda^2$. The wall thickness should be chosen properly to consider the wall crystalline structure and the force field due to all molecules within that structure.

In this study we consider the Face Centered Cubic (FCC) fixed lattice structure at various orientations, and assume electrically neutral surfaces whose molecules interact via the 6-12 Lennard-Jones (L-J) potential. Fig. 1 shows the schematics of the unit FCC fixed lattice solid wall with its atomistic positions and molecular separation length scales. If the (1,0,0) plane faces the fluid, a single FCC structure would occupy a volume of $(0.54)^3\ nm^3$ and contain only 14 molecules. Due to the cut-off distance of the L-J potential ($1.08nm$), one needs to model the walls using at least two layers of FCC structure, which include 23 wall molecules within $2\times(0.54)^3\ nm^3$ volume and will cover only $(0.54)^2\ nm^2$ surface area. Considering the example of the $3.24nm$ height channel for argon flow at $T=298K$ and $P=202kPa$, the total number of molecules required to model both walls (area of $2\times32.4\times32.4nm^2$) is 36,603 (Table 1). One must note our choice of the artificially large pressure of $202kPa$. A similar calculation at one atmosphere would require simulation of 708 argon molecules and 145,203 wall molecules. Therefore, straightforward MD simulations of gas flows suffer from the overwhelmingly large number of wall molecules, which unnecessarily require large computational memory.

In order to develop the smart wall model (SWM) we first formed several layers of FCC wall structures with (1,0,0) plane facing the fluid. We evaluated force interactions between a cluster of these FCC structures and a single molecule approaching to this cluster with various angles of incidence and target locations. Utilizing structure of the FCC crystal and the cutoff distance for the L-J potentials, we were able to develop a truncated molecular wall module that accurately represents the force field on an approaching molecule due a semi infinite half plane. The molecular structure of the resulting SWM, consisting of only 74 wall molecules, is shown in Fig. 2. The centerline of the model

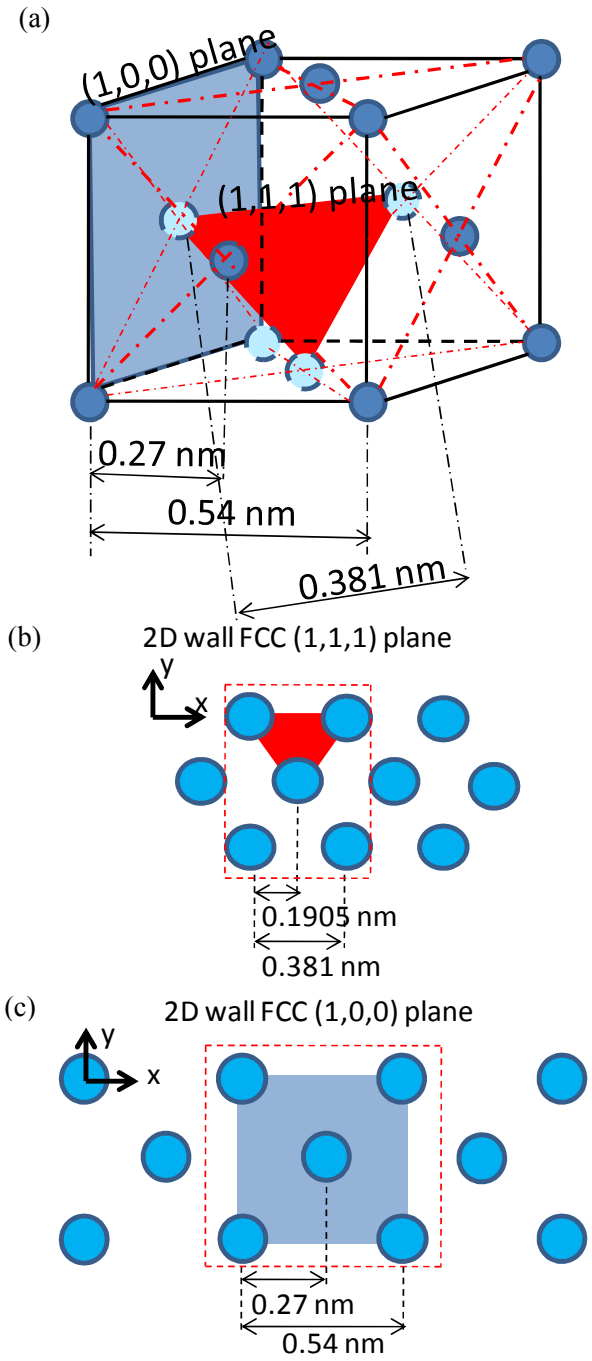



Figure 1: (a) The schematic of the unit FCC fixed lattice for solid walls. Modeling of two-dimensional FCC walls corresponding to the (1,1,1) (b) and (1,0,0) (c) planes.

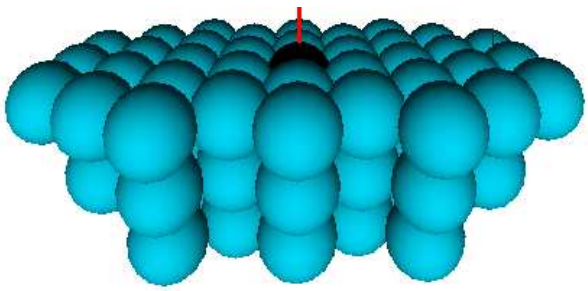


Figure 2: Schematics of the wall surface for optimized gas/wall interaction model for three-dimensional MD simulations. The line represents the center line of the model.

and the center molecule are also shown in the figure. Any gas molecule approaching the SWM targets the basic FCC structure immediately around the centerline. We still apply the aforementioned cut-off distance to calculate the force field properly. Otherwise the molecules within one side of the SWM could falsely bias the force calculations due to the motion of the approaching gas molecules, and/or motion of the surface. The SWM structure, consisting of 74 wall molecules, is formed once and maintained in the computer memory as a basic unit. When a gas molecule is about to enter into the force penetration region ($3\sigma$) of walls, this basic unit, conforming exactly to the crystalline structure of the surface, is placed on the surface. In the case of moving walls, the desired tangential velocity is imposed on the wall molecules according to the wall speed, simulation time and the initial configuration of the wall crystalline structure.

## Two-dimensional versus three-dimensional wall models

In order to assess the differences between two- and three-dimensional simulations, we developed two-dimensional wall models shown in Figs. 1(b) and (c) by utilizing the (1,0,0) and (1,1,1) planes of the basic FCC structure. Similar two-dimensional molecular models were developed and utilized earlier to simplify the MD computations. The smart wall models corresponding to two-dimensional configurations contain 14 and 18 molecules for the (1,0,0) and (1,1,1) planes, respectively. Since two-dimensional simulations require relatively small number of wall molecules, impact of SWM for two-dimensional (2-D) models is not as extensive as in three-dimensional (3-D) simulations.

An important aspect of the three- versus two-dimensional MD simulations is the differences between the wall force fields. In Fig. 3 we show the force fields on a single molecule approaching the 2-D and 3-D walls directly on the center-line of the wall molecules. The 2-D FCC walls with (1,0,0) plane induces the least amount of force on the approaching molecule, while the 2-D FCC wall with (1,1,1) plane has slightly larger influence. None of the two-dimensional model force fields can induce the force due to the three-dimensional model. Therefore, it is necessary to investigate the effects of these wall force fields on the two- and three-dimensional simulations.

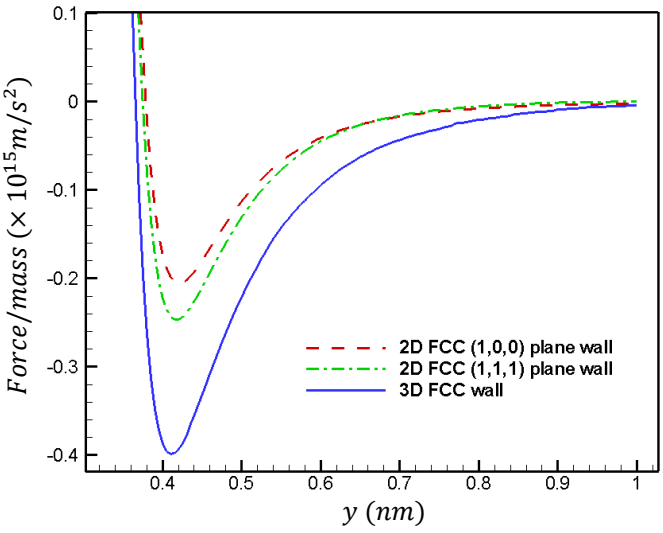



Figure 3: Comparisons of wall force fields for two-dimensional FCC (1,0,0) and (1,1,1) planes and three-dimensional FCC (1,0,0) plane for a fluid molecule approaching the wall through the center line of the wall molecule ($\varepsilon_{wf}/\varepsilon_{ff}=1$ is assumed).

## MD simulation details

We consider flow of argon gas between two infinite parallel plates that are a distance $H$ apart, and moving in opposite directions with a characteristic velocity corresponding to $U_w = M\sqrt{\gamma k_b T/m}$, where $M$ is the Mach number, $\gamma$ is the adiabatic index from kinetic theory (5/3 for monatomic molecules such as noble gases), $k_b$ is the Boltzmann constant ($1.3806\times10^{-23}\ JK^{-1}$), $T$ is the temperature, and $m$ is the molecular mass of wall molecules. The mass for an argon molecule is $m=6.6337\times10^{-26}kg$, its molecular diameter is $\sigma=0.3405nm$ and the depth of the potential well for argon is $\varepsilon=119.8\times k_b$. For simplicity, we utilized the same molecular characteristics for wall molecules. Periodicity boundary conditions are applied in the axial ($x$) and lateral ($z$) directions. A typical simulation domain is shown in Fig. 4. Both plates are maintained at the same temperature, $T_w$=298$K$. The number density of the gas molecules at given temperature and atmospheric pressure ($101kPa$) is equal to $2.69\times10^{25}m^{-3}$.

We performed MD simulations with the isothermal ensemble (NVT) by utilizing (6-12) Lennard-Jones potential

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

for the intermolecular interactions. Formally, all interactions between the nonbonded particles have to be calculated. Since the Lennard-Jones potential vanishes at larger $r_{ij}$ (distance between particles $i$ and $j$), only the interactions with particles within a

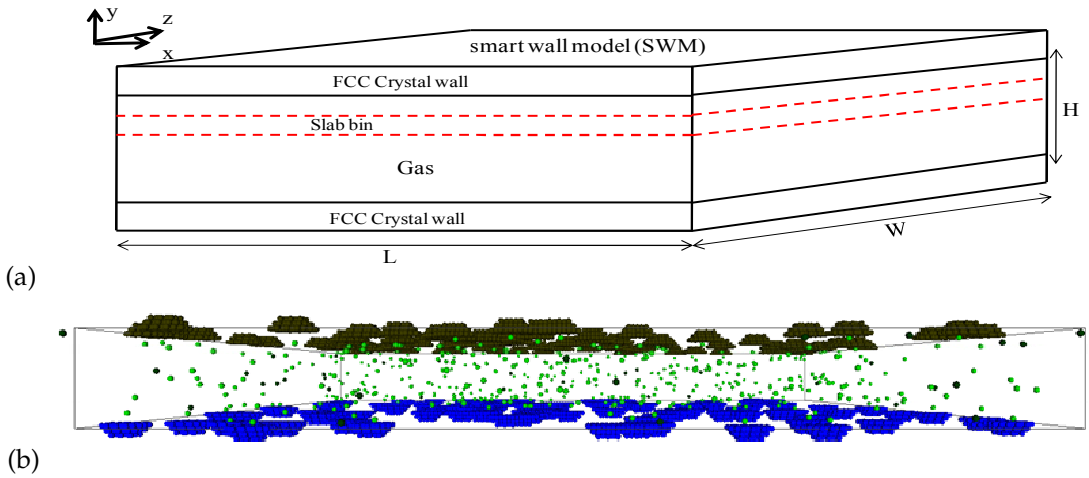



Figure 4: Schematics of the simulation domain and the slab bins used for data analysis (a). Snapshot of three-dimensional SWMD gas flow (b).

certain cutoff radius $r_c$ need to be calculated. Therefore, the intermolecular interaction forces were truncated and switched to zero at a cut-off distance of $1.08nm$, which is approximately at $3\sigma$. Our algorithm utilizes the well known link cell method to handle the particle-particle interactions [19]. In this study, we utilized the potential strength for gas/wall interactions to be the same with that of gas/gas molecular interactions. Thus, we investigated flow of argon gas confined between classical FCC solid walls having the same molecular properties of argon (i.e., $\sigma_{\text{wall}} = \sigma_{\text{argon}}$ and $\varepsilon_{\text{wall-argon (wf)}} = \varepsilon_{\text{argon-argon (ff)}}$). Assuming only van der Waals interactions between gas and wall molecules, the gas/wall interactions are defined using the 12-6 Lennard-Jones potentials. This model is applicable to *any* FCC solid wall with some modifications in the $\sigma_{\text{wall}}$ and $\varepsilon_{\text{wf}}$ values. The wall value is important in definition of the cutoff distance for intermolecular interactions ($\sim 3\sigma$ for the Lennard-Jones model), while $\varepsilon_{\text{wf}}$ is the potential-well depth for gas/wall interactions.

The smart wall algorithm utilizes the fact that gas/wall interactions are limited by the cutoff distance. Therefore, the number of wall molecules needed to give accurate results is a function of the crystal structure of the selected wall model and the cut off distance only. The potential well depth, $\varepsilon_{\text{wf}}$, does not affect the SWMD. However, variations in the $\varepsilon_{\text{wf}}/\varepsilon_{\text{ff}}$ ratio change the gas/wall molecule interaction strength (i.e., wall wettability). Therefore the velocity and density distributions shown in this work are unique to the $\varepsilon_{\text{wf}}/\varepsilon_{\text{ff}} = 1.0$ case. The results will be affected by variations in the $\varepsilon_{\text{wf}}$ value. Since the primary objective of our manuscript is the introduction of the SWMD algorithm, detailed investigations of flow physics as a function of the $\varepsilon_{\text{wf}}/\varepsilon_{\text{ff}}$ ratio will be presented in future studies.

We followed the time evolution of a set of interacting particles by numerically solv-

ing the equations of motion from Newton's law for classical multibody systems. For the steady state constant temperature non-equilibrium MD simulations, Nose-Hoover thermostat [20] with relaxation time $\sim 0.2ps$ was utilized to maintain the system's temperature at 298 K. We use the velocity Verlet algorithm for time integration [11] with characteristic time $\tau = \sigma\sqrt{(m/\varepsilon)} = 2.16\times10^{-12}s$, and the simulations used $4fs$ ($\sim 0.002\tau$) time steps. Simulations started from the Maxwell-Boltzmann velocity distribution for gas molecules, and ran $10^6$ time-steps ($4ns$) to reach a steady state, after which, another $2\times10^6$ time steps ($8ns$) were performed for time averaging. Longer time averaging has also been performed to confirm convergence of the density and velocity profiles to the steady state. Particularly, the simulation times are compared with the mean collision times (predicted by the ratio of the mean free path $\lambda$ to the mean thermal speed $c_m = \sqrt{(8RT/\pi)}$) to result in a state amenable for time or ensemble averaging. Density and velocity distribution in the fluid is obtained using various sizes of slab bins numbered parallel to the walls, as shown in Fig. 4(a). In order to obtain the same $Kn$ value in various height nano-channels under isothermal conditions, we adjusted the base pressure and hence the number density in the simulations. As a result, we were able to maintain $Kn \approx 10$ flow in all simulations, while the affects of wall force field is evaluated for different channel heights. More detail on the specific simulation conditions will be supplied when we discuss the effect of the domain size and periodicity on the simulations. A snapshot of the three-dimensional SWM in an actual MD simulation is shown in Fig. 4(b). Our implementation of the SWM enables simultaneous utilization of the necessary number of wall structures within the domain.

## 3 Two-dimensional simulations

In this section we present the velocity and density profiles for nano-scale confined gas flow at $Kn = 10$ obtained using two-dimensional MD simulations. We utilized the two-dimensional (1,1,1) FCC model, since the wall force field using this model is more dominant than that of the (1,0,0) plane (Fig. 3). Two sets of simulations for $Kn = 10$ are performed using $H = 5nm$ and $H = 10nm$. In order to fix the shear rate we utilized $U_w = 0.6M$ and $0.3M$ in the $H = 5nm$ and $H = 10nm$ channels, respectively. The base temperature was assigned as 298 K and pressure was set to $130kPa$ and $65kPa$ in 5 and $10nm$ height channels, respectively. Both simulations utilized 268 gas molecules with $600nm$ channel length. The channel height is determined from the center lines of wall molecules on the top and bottom surfaces. Because of this definition, $\sigma/2$ distance from each wall is penetrated by wall molecules. The channel height is divided into 100 equally spaced bins, resulting in bin sizes of $0.05nm$ and $0.1nm$ for the $H = 5nm$ and $H = 10nm$ channels, respectively. Considering the bin sizes and molecular diameter, the wall molecules penetrate into approximately 5 and 2 bins for the $H = 5nm$ and $H = 10nm$ cases, respectively.

Velocity profiles within half of the channels are shown in Fig. 5. Particularly the figure shows the relative dimensions of the gas and wall molecules. For the $H = 5nm$ and

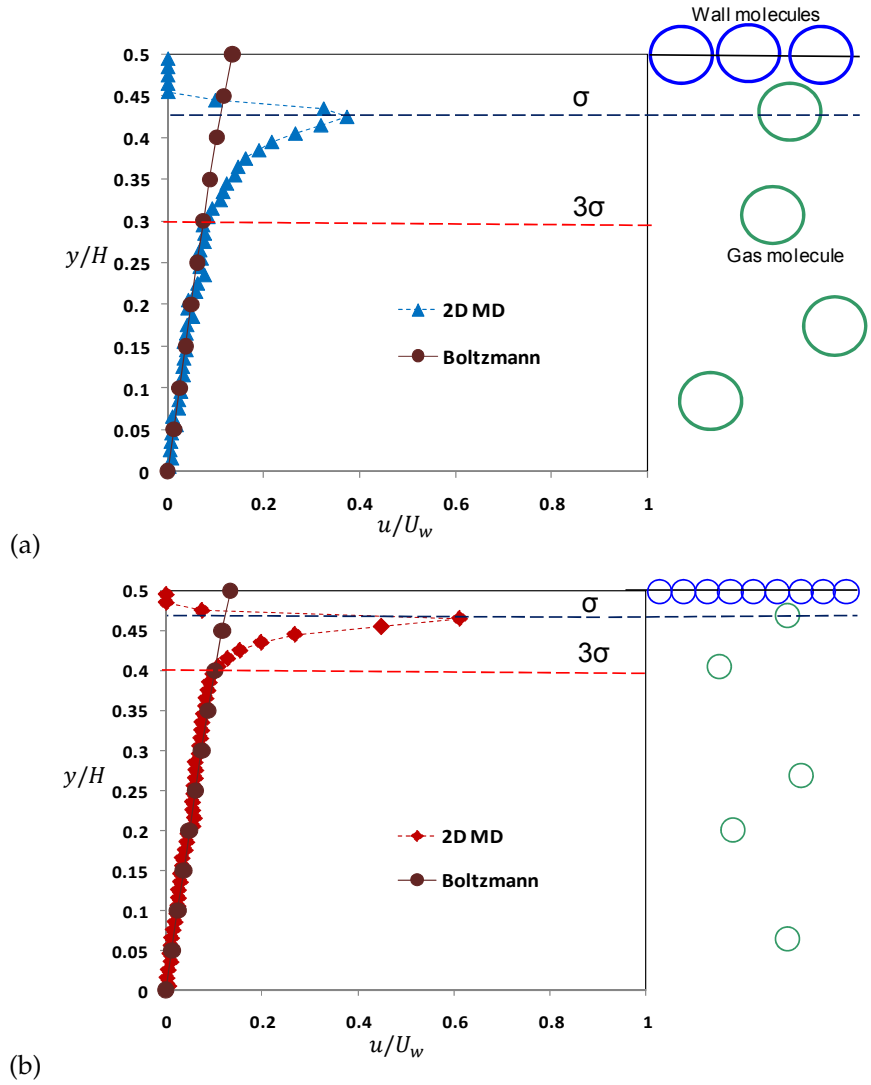



Figure 5: Comparison between the linearized Boltzmann solution and two-dimensional MD gas flow simulations with the smart wall model using the (1,1,1) plane. (a) Velocity profiles in a $5nm$ channel ($U_w = 0.3M$), and (b) $10nm$ channel ($U_w = 0.6M$). Both cases correspond to $Kn = 10$. Scales of gas and wall molecules and the cutoff distance are also shown.

$H = 10nm$ channel cases, the $3\sigma$ cut-off distance covers $2/5^{\text{th}}$ and $1/5^{\text{th}}$ of the channel, respectively. Velocity profiles from the linearized Boltzmann equation solutions at $Kn = 10$, adopted from [9], are also shown in the figure. The Boltzmann equation solutions assume rarefied gas region bounded in $-0.5 \leq y/H \leq 0.5$. The velocity profiles for both cases agree outside the force cut-off distance from the walls. However, there are distinct changes within the velocity profiles in the near wall region. These effects, due to the wall force field, are neglected in kinetic theory solutions.

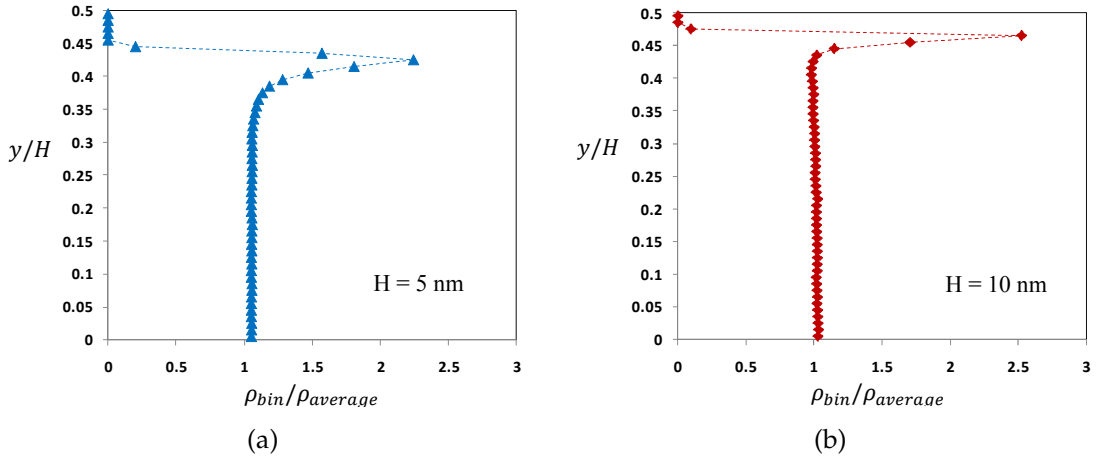



Figure 6: Density profiles within a $5nm$ (a) and $10nm$ (b) channel at $Kn=10$.

The corresponding density distributions are shown in Fig. 6. Due to the blockage of wall molecules in the first few bins, gas density in these bins is rather small. However, the density increases rapidly near the walls, due to the wall force field. Unlike the well known density layering effects experienced in liquid molecules near the walls, the gas density exhibit a single density peak that decay and converge to the mean gas density in the middle of the channel.

## 4 Three-dimensional simulations

The two-dimensional results presented in the previous section cannot utilize the correct wall force field induced by the FCC (1,0,0) plane. In this section we present the velocity and density profiles using three-dimensional simulations to address effects of the proper force field and three-dimensionality on the flow. However, we will first present results of a systematic study on the effects of the simulation domain size and periodicity condition.

### Domain size and periodicity effects

Gas flows evolve through intermolecular collisions, with mean free path being a characteristic length scale of these interactions. Although we are interested in the free molecular flow regime, the Knudsen number is finite. The Knudsen number can be interpreted as the ratio of the gas/surface to gas/gas collision events [1]. As a result, intermolecular collisions for $Kn=10$ flow is about $1/10^{\text{th}}$ of the gas/wall interactions. Given the fact that intermolecular collisions cannot be neglected, effects of the periodic boundary conditions applied on the axial and lateral directions and the domain size need to be quantified. In order to establish this we investigated $Kn=10$ flow in a nano channel with $H=3.24nm$. The simulation parameters correspond to $\lambda=32.4nm$, $P=202kPa$, $T=298K$,

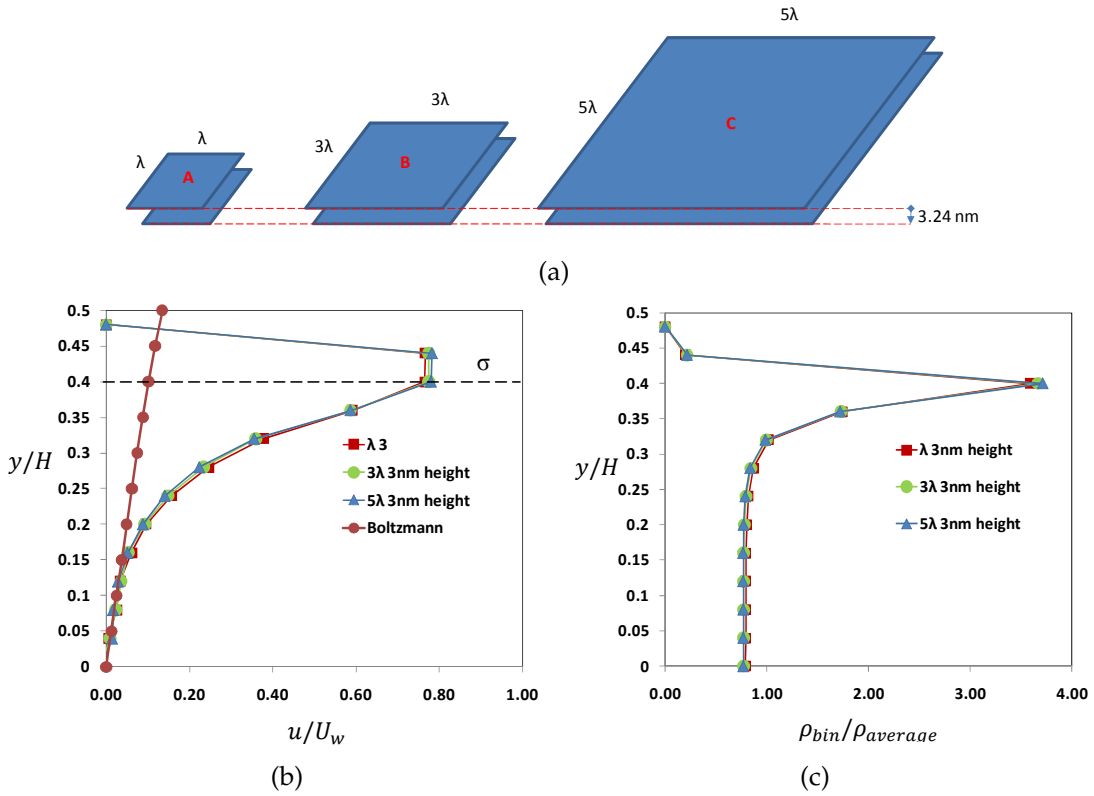



Figure 7: Sizes of the simulation domains with different channel lengths and widths with a fixed channel height (a). Length and width of the each channel are the same for each case and equal to $32.4nm$, $97.2nm$, and $162nm$ for $\lambda\times\lambda$, $3\lambda\times3\lambda$, and $5\lambda\times5\lambda$ domains, respectively. Comparison of the velocity profiles (b) and the density profiles (c) in different sized domains.

and wall velocity of $U_w = 64m/s$ ($0.2M$ flow). Three different simulation domains with $\lambda\times\lambda$, $3\lambda\times3\lambda$, and $5\lambda\times5\lambda$, in the axial and lateral dimensions are utilized (corresponding to $32.4\times32.4nm^2$, $97.2\times97.2nm^2$ and $162\times162nm^2$). The schematics of these flow domains as well as the velocity and density profiles from these simulations are shown in Fig. 7. We observe that the results are unaffected by the domain size, and the $\lambda\times\lambda$ domain dimension in the axial and lateral directions are adequate for our three-dimensional simulations. Due to the unusually small channel height, the velocity profile in the nano-channel is affected mostly by the wall force field. The velocity field obtained from the Boltzmann equation solution is valid only within a very small region near the channel center. The density profiles also exhibit density increase near the walls, and the density reaches to its channel average value within approximately $2\sigma$ distance from the walls. Changes in the gas density seem to be far more dominant than the two-dimensional results, driven by the differences between the two- and three-dimensional wall force fields.

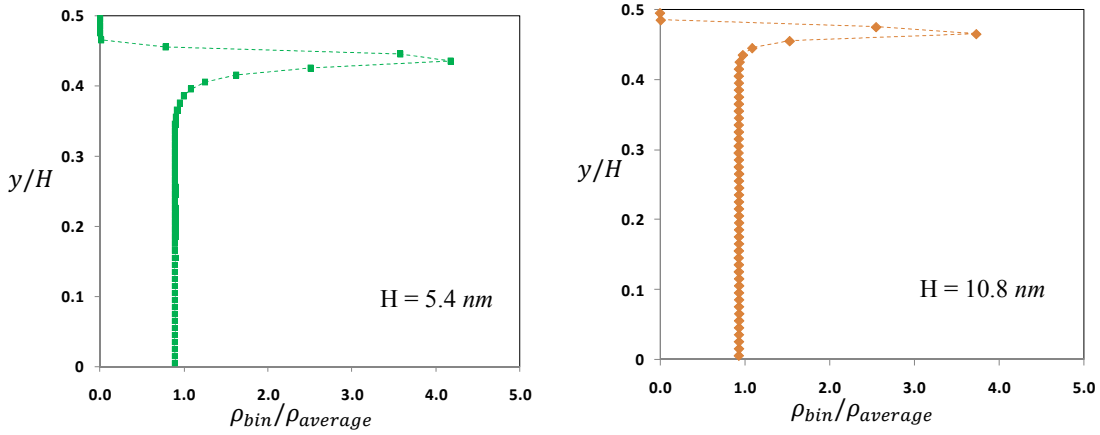
Before we end this section, we revisit Table 1 to discuss the computational impact of the SWMD. The classical MD would be overwhelmed by the number of wall molecules,

which would increase from 36,603 for $\lambda \times \lambda$ simulations to 903,003 for the $5\lambda \times 5\lambda$ case. However, increase in the number of gas molecules is rather moderate, changing from 177 to 4425 for these two cases. The impact of the SWMD is in the treatment of wall molecules, where our code utilized only 74 wall molecules irrespective of the domain size. Although SWMD is a simple innovation, it enables MD simulations of gas flows in arbitrarily large domains, where the computational load is solely dictated by the number of gas molecules.

### 4.1 Velocity and density profiles

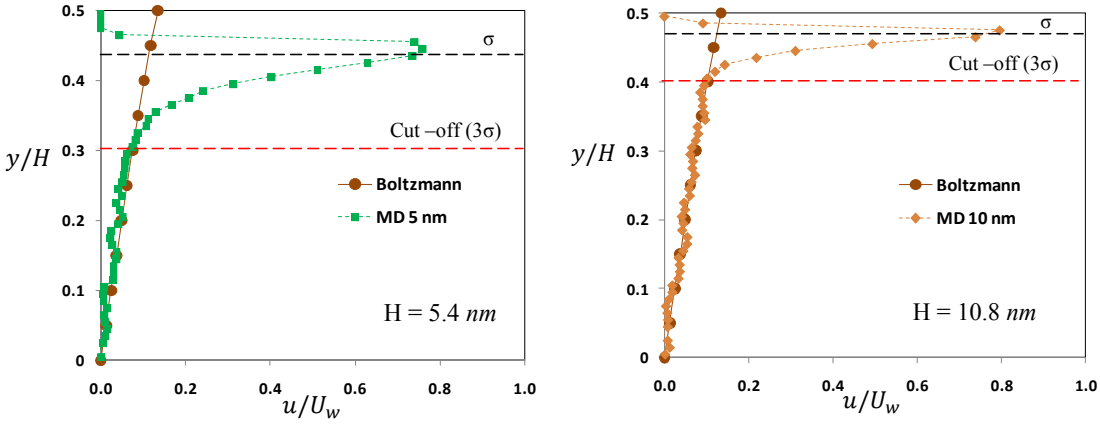
In this section we present the velocity and density profiles obtained from three-dimensional simulations performed in $\lambda \times H \times \lambda$ domains. In order to compare our results with the two-dimensional simulations, we modeled linear Couette flow at $298K$ in $H = 5.4nm$ and $H = 10.8nm$ channels. In order to maintain the flow at $Kn = 10$, pressure was set to $120kPa$ and $60kPa$ in 5.4 and $10.8nm$ height channels, respectively. Three-dimensional simulations were performed using a constant wall velocity of $M = 0.2$. This wall speed was low enough to ensure shear rates that resulted in linear response of the gas slip velocity (This phenomena was originally discussed in [21] for liquid flows). The resulting density profiles, obtained using 100 bins across the nano-channels, are shown in Fig. 8. Increased gas density near the walls is observed in both cases. In comparison with the two-dimensional results, density increase in three-dimensional simulations is more dominant. In fact, comparison between two- and three-dimensional results shows that the amount of density accumulation is up to two times larger in three-dimensional simulations for similar conditions in two-dimensional simulations. This is due to the influence of the force field in three dimensional walls. In future studies we plan to investigate the structure of the density profile near the surface as a function of the gas/wall interaction strength ratio.

In Fig. 9 we present the velocity profiles obtained in three-dimensional simulations along with the results of the Boltzmann equation solution. The MD results agree with the Boltzmann solution in the bulk of the channel. However, effects of the wall force field are felt within $3\sigma$ distance from the walls. For the $H = 5.4nm$ channel, these regions cover 40% of the flow domain, while it covers only 20% of the domain for the $10nm$ channel. Overall, there are significant differences between the velocity profiles of the two- and three-dimensional simulations. Especially, comparison of near-wall velocity field shown in Figs. 9(a) and 7(b) indicate significant differences. In order to asses the velocity profile within the near wall region we present in Fig. 10 the velocity profiles obtained for $Kn = 10$ flow in various channel heights and pressures. All near-wall velocity profiles overlap within the $3\sigma$ region of the wall. It is noteworthy to observe that actual gas velocity near the wall is about $0.8U_w$. Not accounting for the wall force effects, kinetic theory predicts gas velocity of $0.134U_w$. Apparently the wall force field decreases velocity slip on the wall. In future studies we will address the effects of gas/wall interaction strength ratio ($\varepsilon_{\mathrm{wf}}/\varepsilon_{\mathrm{ff}}$), which was set equal to 1 in this work.




(a) (b)

Figure 8: Density profiles for $Kn=10$ flow in $5.4nm$ (a), and $10.8nm$ (b) height channels.




(a) (b)

Figure 9: Velocity profiles in $Kn=10$ flow for $5.4nm$ (a), and $10.8nm$ (b) height channels, and the predictions from the Boltzmann equation solutions.

## 5 Conclusions

Molecular dynamics simulations of gas flows are overwhelmed by the number of wall molecules compared to the gas molecules. This has limited the use of MD in nano-scale gas transport problems. In this manuscript we introduced a smart wall molecular dynamics algorithm (SWMD), which models three-dimensional FCC walls in the (1,0,0) plane using only 74 wall molecules. This is a simple, yet important development, which allowed us to simulate gas flows within arbitrarily large domains. Within the current

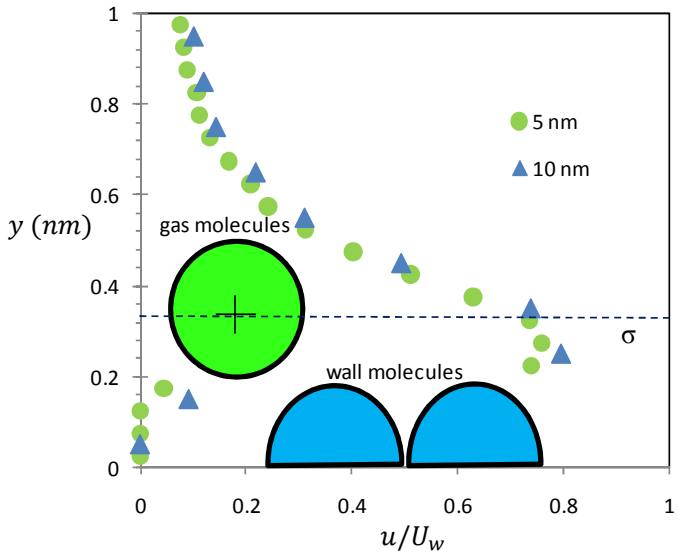



Figure 10: Dimensionless velocity profile within the wall force penetration region at $Kn=10$ and $\varepsilon_{wf}/\varepsilon_{ff}=1$.

implementation, the computations are dominated by the number of gas molecules and their interactions with walls are modeled using the 74 molecule wall stencil, resulting in significant memory savings in computations. Using the SWMD, we were able to assess the effect of domain size and the periodic boundary conditions on gas flows. We have formally shown via three-dimensional MD simulations that one mean free path length is adequate to impose periodicity boundary conditions. To our knowledge, MD simulations of gas flows in such large flow domains have not been attempted before.

Presence of the walls creates an additional length scale based on the Lennard-Jones force field near the walls. This is typically $3\sigma$ in the parametric regime studied here. Therefore $3\sigma$ region near the walls becomes a critical length scale that admits deviations from the kinetic theory. Our SWMD results have shown increase in the gas density and sudden change of the velocity profiles within this region. Kinetic theory solutions based on the Boltzmann equation neglect the wall force field effects, and hence, cannot predict this density increase and the change in the velocity profile. We have shown that the velocity profile within the interface region exhibits self similar behavior regardless of the channel height (provided that $H>6\sigma$ ). Overall, the slip velocity is over predicted using kinetic theory solutions.

We have also shown differences between the two- and three-dimensional simulation results. Especially the density buildup and the velocity profiles near the walls are different due to the differences in the wall force field. In addition, there aren't any equivalent geometrical wall description and wall force fields between the two- and three-dimensions. Therefore, two-dimensional MD is not suitable for full description of nano-channel gas flows.

Our future studies will include systematic investigations of the density build-up and the velocity profiles as a function of the Knudsen number and the gas/wall interaction strength ratio. Further insights could be gained by investigating components of the stress tensor that will enable evaluation of pressure and shear stress, and by relating these to the results from the kinetic theory predictions.

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