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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, λ, 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 λ) 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=6.48nm height channel under standard conditions (λ_{argon}=64nm) 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, 3σ). 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 12.75σ in height, by assigning periodic boundary conditions along the channel length and width of 13.6σ and 5.1σ, 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].