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Atomistic-continuum hybrid simulations for compressible gas flow in a parallel nanochannel

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ABSTRACT

An atomistic-continuum hybrid method is proposed to simulate the compressible gas flow in nanochannel. Based on the domain decomposition method, the computational region is divided into two parts: the atomistic part and the continuum part. In the region near the wall, the molecular dynamics (MD) simulation is used; in the bulk region, finite volume method (FVM) is employed, which also provides necessary information for constructing inlet and outlet boundary conditions of atomistic part. After some validation of the hybrid code, it is used to study the Poiseuille flow in nano-scale channel. Pressures at the inlet and outlet boundaries are both generated as expected, and the pressure gradient is induced along the channel. The velocity and pressure profiles from the hybrid method agree well with full MD simulation. The variations of slip velocity and dimensionless slip length with Knudsen number are also studied, and a linear equation between dimensionless slip length and Knudsen number is obtained.

1. Introduction

The technology in micro/nano-electro-mechanical systems (MEMS/NEMS) has been rapidly developing over the past decades [1–3]. Many phenomena related to fluid flow and heat transfer in these systems are found to be different from that in traditional macro systems, such as velocity slip of fluid flowing over a solid surface [4,5]. Generally, the direct simulation Monte Carlo (DSMC) and molecular dynamics (MD) simulation are used for the simulation of gas flow at micro scale. In the present work, MD simulation is adopted to directly simulate the interaction between fluid and solid.

The micro-/nano- scale Poiseuille flow is probably the simplest case of fluid flow, hence micro-/nano- scale methods are often first adopted to simulate this flow problem. There are several ways to simulate the Poiseulle flow by particle methods. The most popular one is implemented by adding an external driving force to every fluid atom in the channel [6–10]. In this method, periodic boundary condition (PBC) is often used in the flow direction, and the pressure is constant along the flow direction [11] even though the Poiseuille flow can be induced. In order to simulate a fluid flow driven by pressure difference, several new methods have been developed. Li et al. [12] proposed a method named "the reflecting particle method" in which a fictitious membrane was used to filter atoms. The atoms from one direction were allowed to pass the membrane, while those from the other direction were reflected with a specified probability. To generate a pressure gradient along the axial direction of carbon nanotubes (CNT) in which liquid water flows, Nicholls et al. [13] applied different driving forces on water molecules in the control zones at inlet and outlet, respectively, which were adjusted according to the target pressures. The application of a similar method can be found in [14]. Huang et al. [15] used two self-adjusting plates at both ends of a nanopore in order to drive the liquid argon under pressure differences. Instead of applying forces on liquid atoms, they applied forces on both plates. A model named "channel moving" was proposed in [16] to simulate the planar Poiseuille flow. By moving two parallel plates which constitute the channel at the same velocity and fixing a rigid wall at one end of the channel, a constant pressure gradient in fluid was generated.

The above-mentioned methods are mainly applicable to liquid flow. For gas Poiseuille flow, there are not many available methods for generating a pressure gradient along the channel from the literature. Sun and Ebner [17] used a wall at the end of the source region and made the wall compressing the particles as a piston. An appropriate number of particles were inserted into the system according to the Maxwell velocity distribution, which kept the particle density and temperature in source region constant. By setting

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the sink region at the other end of channel at vacuum, a steady-state gas flow was induced under pressure gradient. The deficiency of this method is that pressure at the outlet of the channel is not able to be controlled. To et al. [11] successfully simulated a pressure driven Poiseuille flow by keeping a difference in squared velocity between the molecules which crossed the inlet and outlet faces of the channel.

In this paper, we propose a hybrid MD-continuum method for simulating compressible gas flow in a nanoscale parallel channel, in which by imposing different pressures at the inlet and outlet of the channel the Poiseuille flow can be naturally and successfully simulated. There are two main reasons for using hybrid method for this problem: the first one is that it combines the advantages of both atomistic and continuum methods. The physical characteristics at the gas-solid interface can be captured by the atomistic method while the continuum method can save considerable computational resources. The second one is that with the aid of continuum method, the pressure boundary can be changed to velocity boundary for atomistic region, which is easier to deal with for MD simulation. More details will be given in the next section. Section 2 gives an introduction of our hybrid method. The results of hybrid method and the comparison of results between hybrid method and full MD simulation will be presented in Section 3. Finally, some conclusions are given in Section 4.

2. Hybrid simulations

The schematic of the gas flow through a parallel nanochannel is shown in Fig. 1. Due to the symmetry, only the lower half of the channel is simulated. The simulation domain is decomposed into two regions: continuum (C) region in which finite volume method (FVM) is used, and particle (P) region in which MD simulation is adopted for the atomistic description. The two regions are overlapped and the overlapped one is called overlap (O) region where both FVM and MD are applied. It should be ensured that the results from FVM and MD simulation agree with each other in the O region.

2.1. Molecular dynamics simulation

For gas flow, the Knudsen number (Kn) is very important to distinguish different flow regimes. According to [2,18], when $0.01 < Kn < 0.1$, the gas flow is in the slip-flow regime where the Navier-Stokes equations are still valid, but the tangential slip-velocity and temperature jump at the walls need to be specified explicitly [19–21]. For $0.1 < Kn < 10$, the gas flow falls into the transition flow regime. In this regime, the linear stress-strain relationship fails within the Knudsen layer which is situated roughly one mean-free path from the wall, then particle methods like DSMC [22,23] or MD simulation [24,25] are preferable. In this flow regime analytical models still can be adopted, however, second-order slip model is needed for high Kn cases even though the first-order slip coefficient is widely used in many analytical models for Kn less than 0.1 [17]. This is the reason why in the present paper MD simulation is used to directly describe the interactions between fluid and solid atoms using Lennard-Jones (L-J) potentials, as the Knudsen numbers of the simulated flow is in slip-flow or early transition regimes, from 0.055 to 0.195.

The atomic interactions are described by the following L-J potential:

$$\phi(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{1}$$

where $\varepsilon = 1.67 \times 10^{-21}$ J and $\sigma = 0.341$ nm are the energy and length characteristic parameters for argon, respectively. The Newton's equation of motion is used to update the atoms' accelerations:

$$m_i \frac{d^2 \boldsymbol{r_i}}{dt^2} = -\sum_{j \neq i} \frac{\partial \phi_{ji}}{\partial \boldsymbol{r_i}} \tag{2}$$

where $m_i = 6.634 \times 10^{-26}$ kg is the mass of the ith argon atom. The velocity-Verlet algorithm with a time step δt^{P} of 0.005τ ($\tau = m^{1/2}\sigma\varepsilon^{-1/2}$, where m is the mass of an argon atom) is used to integrate the Newton's equations of motion for P region. All of our MD simulations are performed by using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [26]. The cutoff radius r_c is set to be 3.5σ beyond which the interaction is ignored. The wall is constructed by two layers of atoms forming a face-centered-cubic (FCC) structure with a lattice constant $a = 0.814\sigma$, which corresponds to the configuration of platinum (Pt). During the simulation, all of the wall atoms are fixed. Eq. (1) is also used for the gas-solid interactions, with $\varepsilon_{gs} = 0.54\varepsilon$, $\sigma_{gs} = 0.91\sigma$ [27].

The size of P region is set as $l_x^{\mathrm{P}} = 402.94\sigma$ (including channel length, source region and sink region), $l_y^{\mathrm{P}} = 45.29\sigma$, and $l_z^{\mathrm{P}} = 34.89\sigma$. As shown in Fig. 1, in front of the inlet of the channel a source region of length 35.29σ in x-direction ($-35.29\sigma < x < 0$) is used to adjust the gas density, which guarantees that the gas density at the inlet is $\rho_{\mathrm{in}} = 0.035m\sigma^{-3}$, corresponding to the vapor saturated state at the temperature of system $T = 1.0\varepsilon k_{\mathrm{B}}^{-1}$. The origin of x-coordinate is set to be at the same position as the inlet, and the channel is located at $0 < x < 294.12\sigma$. Behind the outlet of the channel, a sink region situated at $294.12\sigma < x < 367.65\sigma$ is used to reduce the effect of outlet boundary. Whenever an atom arrives at the end of the sink region, it is removed from the system. In

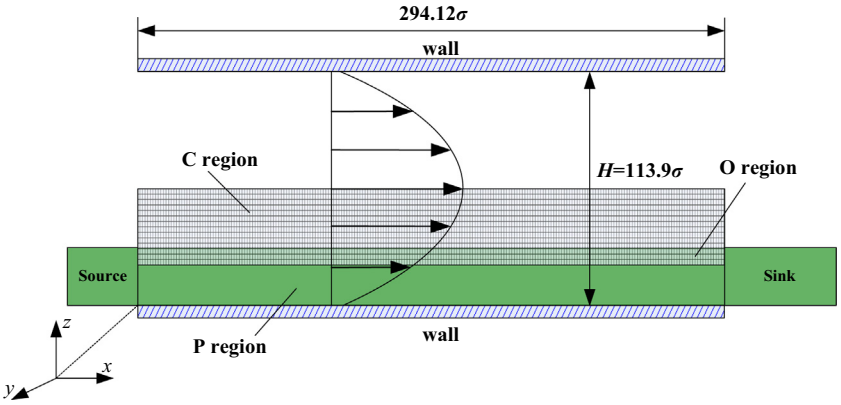

Fig. 1. Schematic of the gas flow through a parallel nanochannel.