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Molecular Simulation of Small Knudsen Number Flows

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Abstract. The direct simulation Monte Carlo (DSMC) method is a powerful particle-based method for modeling gas flows. It works well for relatively large Knudsen (Kn) numbers, typically larger than 0.01, but quickly becomes computationally intensive as Kn decreases due to its time step and cell size limitations. An alternative approach was proposed to relax or remove these limitations, based on replacing pairwise collisions with a stochastic model corresponding to the Fokker-Planck equation [J. Comput. Phys., 229, 1077 (2010); J. Fluid Mech., 680, 574 (2011)]. Similar to the DSMC method, the downside of that approach suffers from computationally statistical noise. To solve the problem, a diffusion-based information preservation (D-IP) method has been developed. The main idea is to track the motion of a simulated molecule from the diffusive standpoint, and obtain the flow velocity and temperature through sampling and averaging the IP quantities. To validate the idea and the corresponding model, several benchmark problems with Kn ~ 10^{-3}-10^{-4} have been investigated. It is shown that the IP calculations are not only accurate, but also efficient because they make possible using a time step and cell size over an order of magnitude larger than the mean collision time and mean free path, respectively.

Keywords: DSMC, IP, molecular diffusion, time step, cell size.
PACS: 51.10.+y, 02.70.Uu

INTRODUCTION

Numerical schemes can be categorized into two kinds: continuum and particle. For real gas flows, a powerful molecular approach is the direct simulation Monte Carlo (DSMC) method [1] that has been successfully applied to various rarefied gas flows [2], especially hypersonic situations, e.g. the structures of strong shock waves [3], aerodynamic features of reentry vehicles [4]. There is a great interest to extend the DSMC method to other situations not only for understanding the mechanisms and patterns of gas flows at molecular level, but also for more conveniently and physically modeling the microscopic transport process behind macroscopic flow phenomena.

To achieve the goal, an issue that has to be addressed firstly is the cell size and time step limitations of the DSMC method [5, 6]. They become stringent when the temporal and spatial scales of a gas flow are much larger than those of molecular motion.

The time step limitation of DSMC results from a core assumption that decouples molecular motion and collisions in a time step Δt [1]. It is physically reasonable only when $\Delta t < \tau_c$, where τ_c is the mean collision time of molecules. Another essential feature of DSMC [1] is to select collision pairs based on pairs of molecules, which is reasonable only when the distance between a pair of molecules is smaller than the mean free path (λ). In the conventional DSMC method, pairs of molecules are formed within a cell, therefore the cell size needs to be smaller than λ. The values of τ_c and λ are usually very small, e.g. about 2×10^{-10} sec and $6\times10^{-8} m$ for air in the standard condition, respectively. Consequently, it is hard to meet the requirements even for parallel supercomputers, except for relatively large Knudsen number flows where the characteristic scales are comparable to or less than τ_c and λ.

Many efforts were made to relax the time step and cell size limitations of DSMC. One of them tracked the motion of a simulated molecule (simulator) with a stochastic model corresponding to the Fokker-Planck equation instead of the decoupling treatment of molecular motion and collisions [7, 8]. It to certain extent eliminated the sources that result in the limitations of time step and collision-pairs distance in DSMC. Along this way, a critical point is how to evaluate flow velocity and temperature that are necessary to calculate the convective motion and diffusive motion of simulators every time step. In previous studies [7, 8], they were obtained through sampling and averaging microscopic velocities. As pointed out by the authors themselves, "stochastic noise will be the same for the new model and DSMC", and "difficulties due to noise for low Mach number flows can be expected for both methods".

In this paper, we suggest to combine the diffusion approach with the information preservation (IP) method. The IP method [9, 10] was originally proposed to overcome the statistical scatter in DSMC calculating microscale gas flows in MEMS usually in low-speed. IP assigns each simulated molecule two velocities: one is

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microscopic velocity, $c_{k,i}$ like DSMC, and the other is called information velocity, $u_{k,i}$, which can be understood as the collective velocity of a large number of real molecules represented by a simulator. In conventional IP method, molecular motion is tracked based on $c_{k,i}$ following the same steps as DSMC, and $u_{k,i}$ is transported along with molecular motion. When a simulator encounters a computational boundary during its movement, $u_{k,i}$ takes the boundary value. When two simulators collide, their information velocities are exchanged according to the corresponding models. The flow velocity is obtained through sampling and averaging the information velocities, which avoids the statistical scatter arising from the random part of the microscopic velocities. The IP method has been successfully applied to many situations, e.g. unidirectional flows [9, 10], microchannel flows [11, 12], and micro plate aerodynamics [13, 14]. All of them exhibited a good agreement with exact solutions or measured data available. A recent advancement of IP was a clear theoretical verification that was based on Maxwell's equation of transfer and established the governing equation of information quantities [15-17].

Briefly speaking, our main idea is to track the motion of simulated molecules in a diffusive view, and obtain the flow velocity and temperature through the IP quantities. In this paper, a diffusion model in consistence with the IP method is described. Prior to it, the Langevin equation is briefly reviewed that is a basis to set up the diffusion model. Then several benchmark problems with small Knudsen numbers are calculated using the present IP method and the IP results are verified in comparison with the DSMC and Navier-Stokes solutions.

THE LANGEVIN EQUATION

It is well known that the Langevin equation was originally invented to explain the Brownian motion of dust particles, which can be written as [18-20]

$$\frac{dr_i}{dt} = c_i \,, \tag{1a}$$

$$\frac{dc_i}{dt} = -\zeta c_i + A_i \,, \tag{1b}$$

where r_i and c_i are the particle position and velocity, ζc_i and A_i are the mean and fluctuating forces acted on the particle by the surrounding molecules, $\zeta = k_B T/(mD)$, k_B is the Boltzmann constant, and m, D and T are the molecular mass, diffusion coefficient, and temperature of the ambient fluid, respectively.

Eq. (1) is a stochastic differential equation, and its solution describes the position and velocity evolution of a particle in a probabilistic sense. For locally isotropic cases, Eq. (1) has an analytical solution that was firstly obtained by Chandrasekhar [18]

$$W(R_x, S_x) = \frac{1}{2\pi (FG - H^2)^{1/2}} \exp\left[-\frac{R_x^2}{2F} - \frac{(FS_x - HR_x)^2}{2F(FG - H^2)} \right], \tag{2}$$

with

$$R_x = x - x_0 - c_{x0}\left(1 - e^{-\zeta t}\right)/\zeta \,, \tag{3a}$$

$$S_x = c_x - c_{x0} e^{-\zeta t} \,, \tag{3b}$$

$$F = \frac{k_B T}{m\zeta^2}\left(4e^{-\zeta t} - e^{-2\zeta t} + 2\zeta t - 3\right), \tag{3c}$$

$$G = \frac{k_B T}{m}\left(1 - e^{-2\zeta t}\right), \tag{3d}$$

$$H = \frac{k_B T}{m\zeta}\left(1 - e^{-\zeta t}\right)^2 , \tag{3e}$$

where x_0 and c_{x0} are the initial position coordinate and velocity component in the x direction, respectively.

As discussed in details in [18-20], the Langevin equation (1) not only applies to dust particles, but also many other phenomena. For molecular motion interested here, when time is much larger than τ_c , the force acted on a molecule can also be divided into two parts: mean and fluctuating. As a result, the Chandrasekhar distribution (2) is also suitable to describe the position and velocity evolution of a molecule. A numerical comparison is made in figure 1 for an argon gas in the standard condition. Initially a group of molecules gathered at x=0, with a temperature of 273K and zero flow velocity. We see clearly that the molecular position distributions at two time intervals ($100\tau_c$ and $500\tau_c$) predicted by (2) agree well with the DSMC results.

A DIFFUSIVE INFORMATION PRESERVATION METHOD

In a diffusive viewpoint, molecular motion can be expressed as follows

$$r_{k,i}^{t+\Delta t} = r_{k,i}^{t} + u_{k,i}^{t} \times \Delta t + \Delta r_{k,i}^{D}, \tag{4}$$

where the second and third terms on the right-hand side reflect the convective motion and diffusive motion of a molecule, respectively.

If we employ the Langevin equation to describe the diffusive motion of a molecule, according to the Chandrasekhar distribution (2), we have

$$\Delta r_{k,i}^{D} = \left(-2F \ln \Phi_r\right)^{1/2} \cos\alpha_r + c_{k,i}^{'}(t)\left[1-\exp\left(-\zeta\Delta t\right)\right]/\zeta, \tag{5}$$

$$c_{k,i}^{'}(t+\Delta t) = \left[-\frac{2\left(FG-H^2\right)}{F}\ln\Phi_r\right]^{1/2} \cos\alpha_r + \frac{H\times R_i}{F} + c_{k,i}^{'}(t)\exp(-\zeta\Delta t), \tag{6}$$

where Φ_r and α_r are random numbers uniformly distributed in $[0,1]$ and $[0,2\pi]$, respectively.

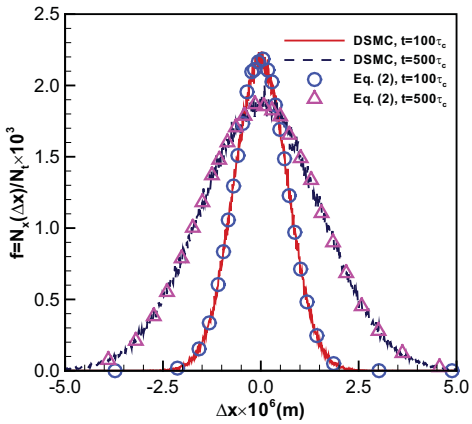


FIGURE 1. Comparison of the molecular position distributions at two time intervals. Symbols: the Chandrasekhar distribution (2); lines: the DSMC results.

This paper suggests a diffusive information preservation (D-IP) method that tracks the motion of a simulated molecule using Eqs. (4-6), calculates the convective motion in Eq. (4) based on the information velocity, and obtains temperature used in Eqs. (5) and (6) through sampling and averaging the information temperature every time step. Similar to the conventional IP method, there are six steps to implement the D-IP method.

1. **Initialization.** Each simulator is initially given a position $r_{k,i}$ (k=1,2,…,N), a thermal velocity $c_{k,i}^{'}$, an information velocity $u_{k,i}$, and an information temperature T_{IP-k} according to the initial conditions of a gas flow.
2. **Molecular motion.** After a time step, simulator k acquires a new position and thermal velocity according to Eqs. (4-6).
3. **Update information velocity and temperature.** After a time step, the information velocity and temperature of a simulator is updated according to the governing equations as follows.

$$\frac{\partial}{\partial t}\left(nmu_i\right) + collective\ movement = -\psi_\eta \frac{\partial}{\partial x_j}\left(nm\overline{u_i c_j}'\right) - \frac{\partial}{\partial x_i}\left(\frac{1}{3}\psi_\eta nm\overline{u_j c_j}'\right) - \frac{\partial p}{\partial x_i} + collisions, \tag{7}$$

$$\frac{\partial}{\partial t}\left[nm\left(3RT_{IP}+u^2\right)\right] + collective\ movement = -\psi_\kappa \frac{\partial}{\partial x_j}\left(3Rnm\overline{T_{IP}c_j}'\right) - \psi_\eta \frac{\partial}{\partial x_j}\left(nm\overline{u^2 c_j}'\right) - \frac{2}{3}\psi_\eta \frac{\partial}{\partial x_j}\left(nmU_j\overline{c_i' u_i}\right) - 2\frac{\partial}{\partial x_j}\left(pU_j\right) + collisions \tag{8}$$

4. **Information velocity and temperature changes due to collisions.** A time step of D-IP is usually much larger than the mean collision time. This means that a simulator will experience enough collisions during it. Therefore, it is assumed that the information velocity and temperature at $t+\Delta t$ is equal to the mean values of its surrounding molecules, i.e.

$$u_{k,i}^{t+\Delta t} = \frac{1}{N_k}\sum_{j=1}^{N_k} u_{j,i}^{t+\Delta t}, \tag{9}$$

$$T_{IP-k}^{t+\Delta t} = \frac{1}{N_k}\sum_{j=1}^{N_k} T_{IP-j}^{t+\Delta t} + \frac{\psi_\eta}{2c_v N_k}\left(\sum_{j=1}^{N_k} u_{j,i}^{t\ 2} - \sum_{j=1}^{N_k} u_{j,i}^{t+\Delta t 2}\right), \tag{10}$$

where N_k is the number of simulators in a neighboring region around simulator k, the region size can be chosen according to the spatial scales and computational accuracy of flows, and c_V is the specific heat at constant volume. The second term on the right-hand side of Eq. (10) is necessary to satisfy the energy conservation and viscous dissipation.

5. **Interact with boundaries.** When a simulator encounters a computational boundary during its movement in a time step, its information velocity and temperature take the boundary values as usual. A criterion whether it interacts with a computational boundary is described in details in Appendix.
6. **Sample and average.** The flow velocity and temperature are obtained by sampling the information quantities of simulators each cell through ensemble average for unsteady cases, and time average for steady cases, i.e.

$$U_i = \overline{u_i}\,, \tag{11}$$

$$T_c = \overline{T_{IP}}\,. \tag{12}$$

The flow number density is calculated using the mass conservation equation:

$$\frac{\partial(nm)}{\partial t} + \frac{\partial(nmU_j)}{\partial x_j} = 0\,. \tag{13}$$

BENCHMAR PROBLEMS

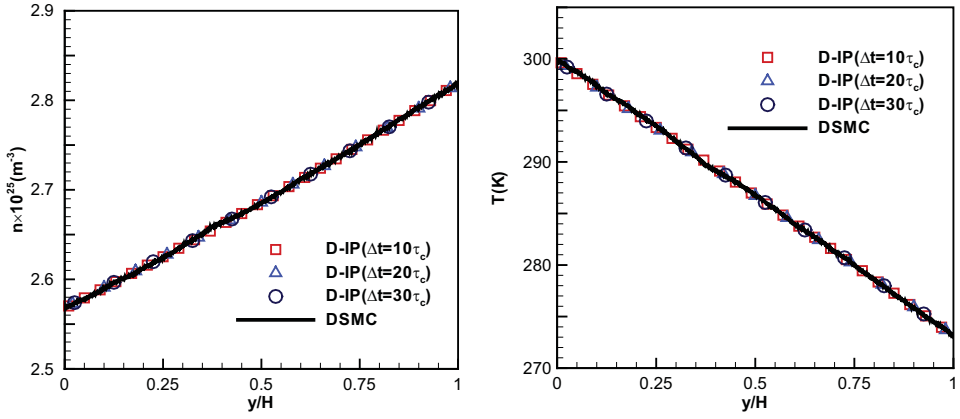
Thermal Couette Flow

Thermal Couette flow is driven by a temperature difference between two infinite and parallel plates. In the present study, the flow medium is argon gas in the standard condition (1atm & 273K), and the bottom and top plates have temperatures of 300K and 273K, respectively, whose surfaces are diffusively reflecting. The distance between the plates $H = 500\lambda$.

Three calculations are performed using the D-IP method, and their computational parameters are given in Table 1. All of them start from a stationary uniform flow field. As shown in Fig. 2, the number density and temperature profiles of D-IP in the three calculations all agree well with that obtained by the DSMC method, so do the values of the heat flux (W/m^2) given in the fourth row of Table 1. Note that in Table 1, the CPU hours of Intel i5 2.66GHz consumed by the D-IP calculations decrease as the time steps and cell sizes increase, and all of them are much less than the CPU hours of DSMC.

TABLE 1. Parameters and results of D-IP and DSMC calculating thermal Couette flow

Parameters	D-IP			DSMC
Δt	$10\tau_c$	$20\tau_c$	$30\tau_c$	$0.3\tau_c$
Δy	10λ	20λ	25λ	0.3λ
q_w (W/m^2)	1.46×10^4	1.45×10^4	1.45×10^4	1.47×10^4
CPU (hr)	0.27	0.1	0.08	21



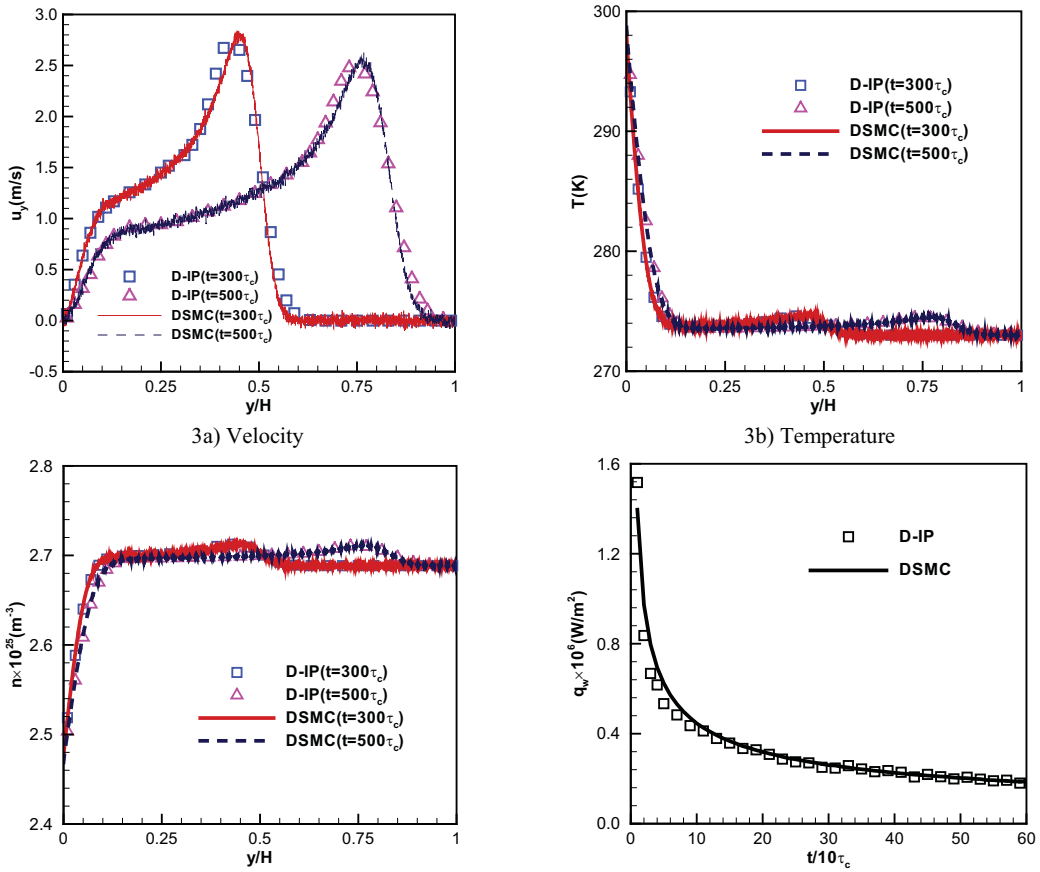
2a) Number density 2b) Temperature

FIGURE 2. Comparison of flow field profiles obtained by D-IP and DSMC for thermal Couette flow (Kn=0.002)

Thermal Rayleigh Flow

In a thermal Rayleigh flow, the stationary plate acquires a temperature increase ΔT_w at the initial time (t=0). This induces an unsteady flow of the gas near the plate. In the present study, ΔT_w = 27K, and the outer boundary is placed 500λ away from the plate to avoid possible backward disturbance during the calculated time interval. The time step and cell size of D-IP are $10\tau_c$ and 10λ, respectively. The other computational parameters are the same as those used in the Couette flow.

Figure 3 shows the flow fields at two moments ($300\tau_c$ and $500\tau_c$), as well as the heat flux versus time, obtained by the D-IP method and the DSMC method. They agree well with each other, except the heat flux at the beginning interval where the time step used in D-IP is too large to resolve the evolving details (Fig.3d).



3a) Velocity

3b) Temperature

3c) Number density

3d) Heat flux

FIGURE 3. Comparison of the velocity, temperature and number density profiles at time of $300\tau_c$ and $500\tau_c$, as well as the evlolution of heat flux, predicted by D-IP and DSMC for the thermal Rayleigh flow.

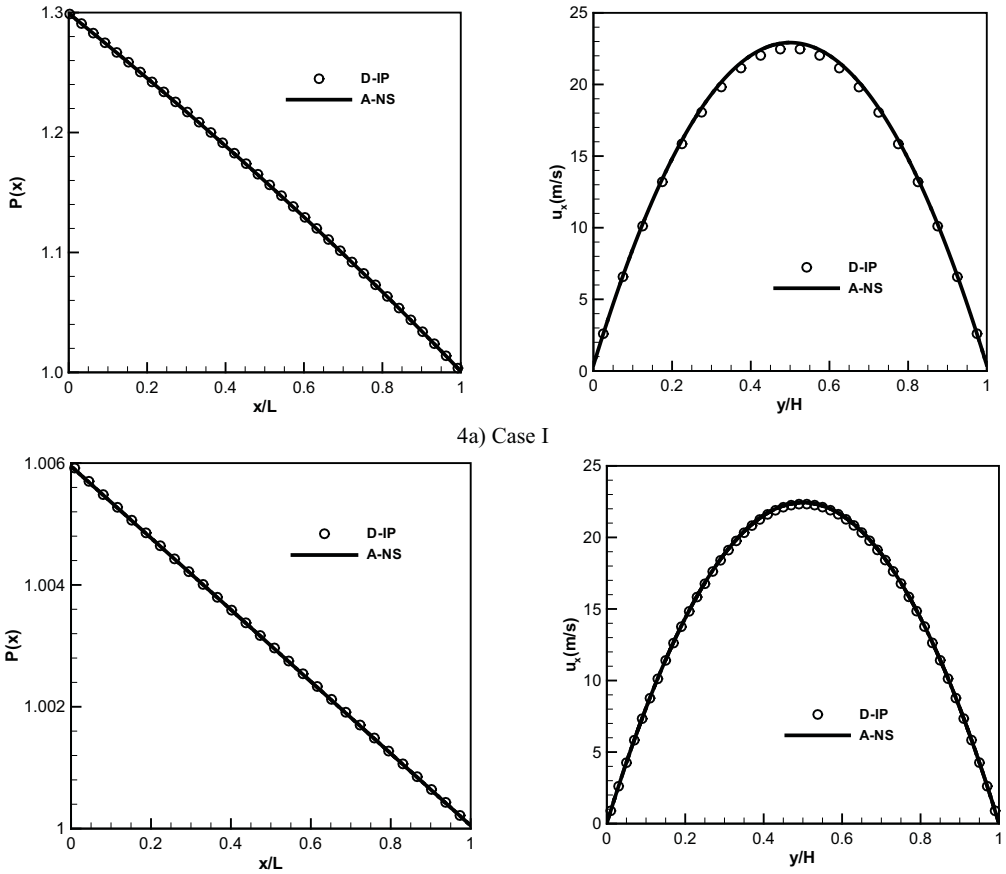
Two-dimensional Channel Flows

A two-dimensional channel flow is a steady flow confined between two finite parallel plates. It is driven by a pressure difference between the inlet and outlet. In the present study, the flow medium is also argon gas, and the ratio of the channel length (L) to its height (H) is 100. The channel walls are difussively reflecting and have the same temperature of 273K. Two cases are investigated, and the corresponding computational parameters are given in Table 2. The outlet pressures for both cases are of 1atm, while the inlet temperatures keep at 273K.

TABLE 2. Compuattaional parameters of D-IP for two-dimensional channel flows

Case	H/λ	L/λ	P_{in} (atm)	Cell number	Time step
I	200	2×10^4	1.3	200×20	$10\tau_c$
II	10000	1×10^6	1.006	56×50	$200\tau_c$

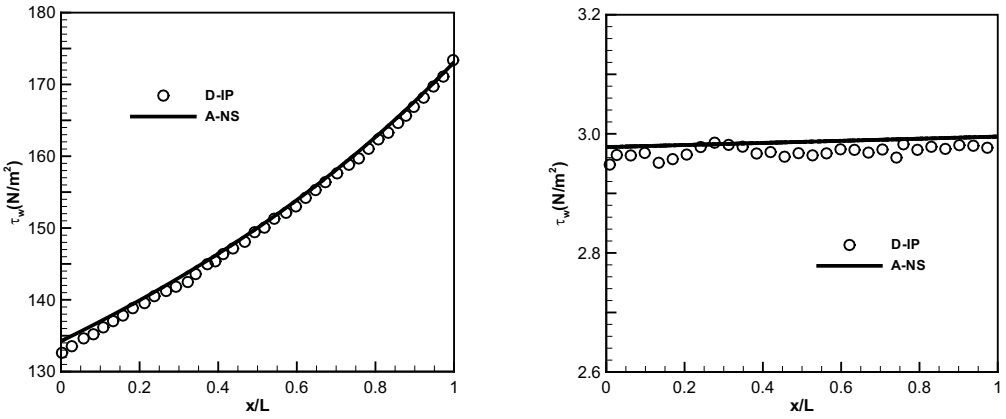
Figure 4 shows the pressure distributions in the streamwise direction and the streamwise velocity profiles obtained by D-IP for the two cases. They agree well with the analytical Navier-Stokes solutions of Arkilic et al [22], so do the shear stress distributions along the channel walls (Fig. 5). Note that the channel length of Case II is about 6cm. This exhibits the D-IP method capable of analyzing gas flows with a common size.



4a) Case I

4b) Case II

FIGURE 4. Pressure distributions along the steamwise direction (left) and streamwise velocity profiles at x/L =0.5 (right) for the channel flows. Circles: D-IP results; lines: analytical Navier-Stokes solutions [22]



5a) Case I

5b) Case II

FIGURE 5. Shear stress distributions along the channel walls. Circles: D-IP results; lines: analytical N-S solutions [22]

CONCLUSIONS

The D-IP method has been developed to relax the limitations of time step and cell size associated with the conventional IP calculations of small Knudsen number flows, and enables us to investigate effectively the mechanisms and patterns of flows at molecular level. For benchmark problems such as thermal Couette flow, thermal Rayleigh flow, and two-dimensional channel flows with Kn ~ 10^{-3}-10^{-4}, the D-IP calculations are not only efficient, but also consistent with the DSMC or Navier-Stokes solutions. It is looking forward to applying the D-IP method to more issues like flow instability and turbulence to promote our understanding of the microscopic nonequilibrium mechanism behind these macroscopic nonlinear phenomena.

APPENDIX: CRITERION ON THE INTERACTION BETWEEN SIMULATED MOLECULES AND A COMPUTATIONAL BOUNDARY

According to the diffusion model, when simulator k has no interaction with a computational boundary during a time step, its new position and thermal velocity after Δt are determined by equations (4) and (6), respectively. Now let us consider an interaction between a simulator and a computational boundary. This consists of two issues. One is to judge whether a simulator interacts with a computational boundary; the other is how to determine the molecular position and velocity after an interaction. The second issue is the same as the conventional IP method, we will focus on the first one.

For the sake of simplicity, an one-dimensional case is considered. For a computational boundary at y=0, there are two situations:

(1) Deterministic interaction. If the position of simulator k after a time step is smaller than zero, it interacts with the boundary during the interval, Δt .

(2) Probabilistic interaction. If the position of simulator k after a time step is larger than zero, it still probably interacts with the boundary during Δt . Our problem can be stated as follows: for a known position $y_0 > 0$ at t, what is the probability $f_{out}(y, y_0)$ in which y is always larger than zero during Δt ?

Such a problem was studied well, e.g. in [21], which gave rise to

$$f_{out}(y, y_0) = \frac{1}{(2\pi F)^{\frac{1}{2}}}\left\{\exp\left[\frac{(y-(y_0+d_{y0}))^2}{2F}\right]-\exp\left[\frac{(y+2\alpha\lambda_B+(y_0+d_{y0}))^2}{2F}\right]\right\}, \tag{A1}$$

where $d_{y0} = c_y'(t)(1-e^{-\zeta t})/\zeta$, $\alpha = 1.46$, $\lambda_B = \sqrt{k_B T/(m\zeta^2)}$, and F is defined by Eq. (3c).

According to the Chandrasekhar distribution (2), the probability from y_0 to y is

$$f(y, y_0) = \frac{1}{(2\pi F)^{1/2}}\exp\left\{\frac{\left[y-(y_0+d_{y0})\right]^2}{2F}\right\} . \tag{A2}$$

Compare the ratio of $f_{out}(y, y_0)$ to $f(y, y_0)$ with a random number uniformly distributed between 0 and 1. If the ratio is less than the random number, the simulator interacts with the boundary during the time interval; otherwise, no interaction.

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