Monte Carlo Modeling of Micro Scale Gas Flows

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ABSTRACT

An information preservation (IP) method has been used to simulate many micro scale gas flows. It may efficiently reduce the statistical scatter inherent in conventional particle approaches such as the direct simulation Monte Carlo (DSMC) method. This paper reviews applications of IP to some benchmark problems. Comparison of the IP results with those given by experiment, DSMC, and the linearized Boltzmann equation, as well as the Navier-Stokes equations with a slip boundary condition, and the lattice Boltzmann equation, shows that the IP method is applicable to micro scale gas flows over the entire flow regime from continuum to free molecular

Keywords: Information preservation method, direct simulation Monte Carlo method, statistical fluctuation, micro scale gas flows, rarefied gas dynamics.

1 INTRODUCTION

There is a great interest to understand in detail the aerodynamics of micro-electro-mechanical systems (MEMS). The characteristic length scale of MEMS is often comparable to the mean free path of molecules, and the Knudsen number, $Kn = \lambda / L$, is no longer small enough to be negligible, where λ is the mean free path of molecules, and L is the characteristic length of flow. Molecular-based numerical schemes, such as the direct simulation Monte Carlo (DSMC) method [1], are more physically appropriate for this kind of gas flows where non-continuum, rarefied gas effect becomes important. In the DSMC method, macroscopic observable quantities, such as velocity and temperature, are obtained through averaging appropriate microscopic properties over a small space region. The simulated results are therefore inherently accompanied with statistical noise due to finite sampling. From equilibrium statistical mechanics, a signal-to-noise ratio in a dilute gas may be written as [2]

$$\phi \equiv \frac{u}{\delta u} = Ma\sqrt{\gamma N}\,, \tag{1}$$

where u is the characteristic velocity of flow, δu is the statistical fluctuation, M is the Mach number, γ is the specific heat ratio, and N is the sample size. Micro-devices often operate at low M, e.g. a typical flow velocity in micro-channel experiments [3] is about 0.2 m/s that corresponds to Ma of 10^{-4}. Relation (1) indicates that if we require the signal is larger in order than the noise, e.g. $\phi = 10$, N has to be 10^{10}. Such an enormous sample size is extremely time-consuming and beyond the capabilities of current computers [4].

There was a consideration [2] that when Ma is small enough for compressibility effects to be negligible, favorable relative statistical errors may be obtained by performing simulations at an increased Ma to a level where compressibility are still negligible. However, this is infeasible for rarefied gas flows interested in MEMS, where the similarity parameters, Ma and Kn, must be satisfied simultaneously. A clear demonstration of this fact was provided by Millikan's measurements of drag of a small sphere over the entire flow regime [5]. The fitting formula of the measured data is dependent on two similarity parameters, Re and Kn. They are equivalent to Kn and Ma due to the relation

$$Kn \sim Ma/\mathrm{Re}\,. \tag{2}$$

The number of similarity parameters is reduced only at extreme situations, i.e. $Kn \to 0$ or $Kn \to \infty$, corresponding to the continuum and free molecular limits, respectively.

An information preservation (IP) method was proposed to analyze micro-scale gas flows [6]. In this method, simulated molecules move through physical space and undergo collisions appropriate to the thermal velocities using the same algorithms and models as the DSMC method, while the macroscopic observable quantities, such as velocity and surface shear stress, are obtained through averaging appropriate physical information carried along with the simulated molecules. The physical information reflects the collective behavior of the enormous number of real molecules represented by each simulated molecule in the DSMC method, and therefore it is not subject to the statistical noise caused by the thermal velocity.

The IP method has been used to simulate many micro scale gas flows [6-13]. This paper briefly reviews IP applications in benchmark problems such as the Couette flows [6,7], Rayleigh flows [6,7], and micro-channel gas flows [13].

2 COUETTE FLOWS

The Couette flow is a steady flow that is driven by the surface shear stresses of two infinite and parallel plates moving oppositely along their own planes. The Knudsen number is defined based on the distance between the plates.

Figure 1 compares the velocity profiles given by the IP method, the linearized Boltzmann equation [14,15], and the Navier-Stokes equations with a slip boundary condition. The velocity at the channel surface ($y/h=0.5$) significantly decreases as Kn increases. The IP profiles are in excellent agreement with the numerical solutions of the linearized Boltzmann equation [15] that are more accurate than the four-moment solutions based on the second approximation [14]. The slip N-S profiles agree with the other three at $Kn = 0.2/\sqrt{\pi}$, but deviate from them as Kn increases.

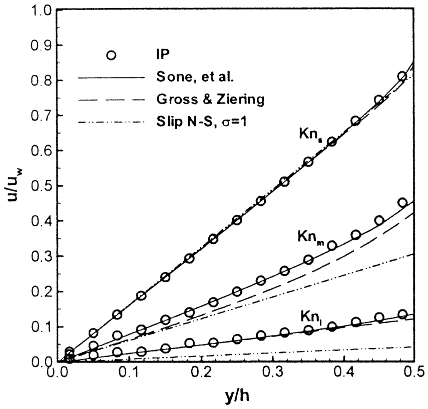


Figure 3. Comparison of velocity profiles in the Couette flow in the transition regime given by the IP method, linearized Boltzmann equation, and slip Navier-Stokes equations [6,7]. $Kn_s = 0.2/\sqrt{\pi}$, $Kn_m = 2/\sqrt{\pi}$, and $Kn_l = 20/\sqrt{\pi}$.

3 RAYLEIGH FLOWS

In the Rayleigh flow, the stationary plate acquires a velocity of u_w in the x direction at the initial time ($t=0$). This impulsive motion of the plate induces an unsteady gas flow. The ensemble average is employed in IP simulation of the unsteady process. The computational domain is between the plate surface and an outer boundary. The specularly reflecting condition is applied to the outer boundary. It is chosen far away from the plate to avoid possible backward disturbance to the gas motion near the plate that is of interest.

Figure 2 shows the relation of the normalized surface shear stress versus time given by various methods, where the normalization factor is the free molecular solution. For a time comparable with the mean collision time τ_c , the DSMC method is employed to give a benchmark solution. Such a calculation, however, is very time-consuming. To reduce statistical scatter in the DSMC results, an enormous sample size of 2×10^8 is used. It takes the CPU hours about 3×10^4 times than required by the IP method. The IP results agree well with the collisionless solution at $t << \tau_c$, with the DSMC results at $t \sim \tau_c$, and with the slip N-S solution at $t > 5\tau_c$.

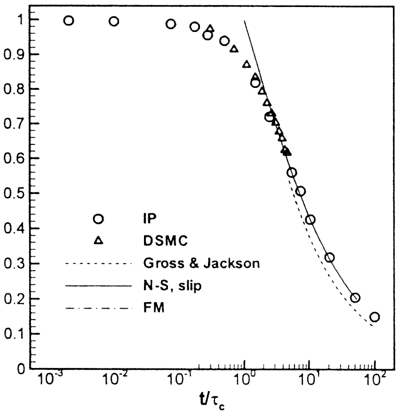


Figure 2. Relation of drag vs time in the Rayleigh flow [7].

4 MICROCHANNEL FLOWS

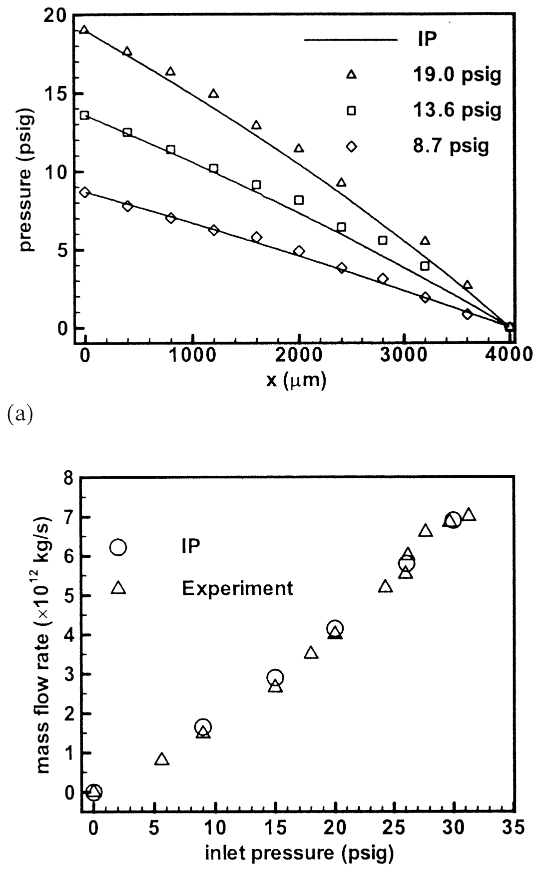
4.1 Experimental micro-channels

In micro-channel experiments performed by Pong et al [16], Shih et al [17], Arkilic et al [18] and Arkilic [19], respectively, the channel width was much larger than the height. This made the span-wise influence neglected, and the flows were simplified as two-dimensional. The degree of rarefaction may be measured by Kn based on the channel height. The Knudsen number at the outlet Kn_O indicated that the experimental conditions [16-19] were in the slip and transition regimes, respectively.

Stream-wise pressure distributions and mass fluxes through micro-channels given by the IP method [13] agreed well with experimental data measured by Pong et al [16], Shih et al [17], Arkilic et al [18], and Arkilic [19], respectively. Comparison of the IP results with the measured data of Shih et al is shown in Fig. 3.

4.2 Short micro-channels

In addition to various experimental conditions, a two-dimensional short micro-channel was investigated over the entire Knudsen regime from continuum to free molecular using the IP and DSMC methods [16]. The micro-channel was 1 μm high and 15 μm long, and the surfaces were assumed to be fully diffuse. The pressure difference between the inlet and outlet led to a stream-wise velocity at order of 10 m/s, which makes DSMC calculations affordable.



(a)

(b)

Figure 3. Comparison of IP results with measured data at experimental conditions of Shih et al (1996): (a) streamwise pressure distributions at three inlet pressures, and (b) relation of mass flux versus the inlet pressure [13].

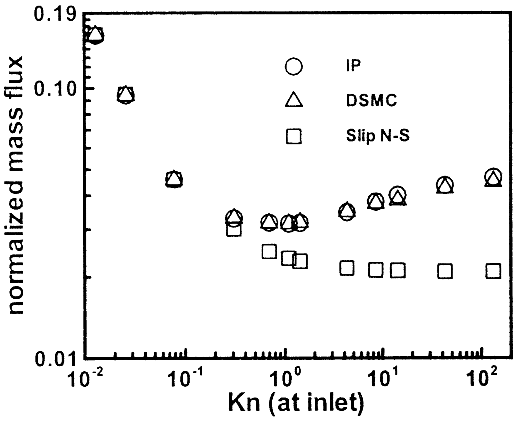


Figure 4. Relation of the normalized mass flux versus the inlet Knudsen number for a short micro-channel [13].

The normalized mass flow rates as functions of the Knudsen number at the inlet, Kn_i are shown in Fig. 4, where the ratio of the outlet to inlet pressure is 0.7, the normalized factor of mass flux is $(\rho_i + \rho_o)v_m H/2$, ρ_i and ρ_o are the inlet and outlet densities, respectively, $v_m = \sqrt{2RT}$ is the most probable thermal speed, and H is the channel height. The IP and DSMC results are in excellent agreement over the entire Knudsen regime, and demonstrate a minimum around Kn_i of 1. This phenomenon was first observed in experiment by Knudsen, and therefore is referred to as the Knudsen minimum. The slip Navier-Stokes solution accords with the IP and DSMC results in the slip regime as $Kn_i < 0.1$, but deviates from them in the transition regime and fails to predict the Knudsen minimum.

In recent lattice Boltzmann (LB) simulation of gas flows through a microchannel [20], the normalized pressure deviation from a linear distribution, $(P - P_\ell)/P_o$, was a positive nonlinear function as $Kn \le 0.2$, where $P_\ell = P_o + (P_i - P_o)(1 - X)$, P_i and P_o are the inlet and outlet pressures, respectively, $X = x/L$, and L is the channel length. For $Kn \ge 0.2$, the LB results showed that $(P - P_\ell)/P_o$ became negative.

The IP and DSMC methods are employed to investigate this phenomenon [21]. The computational parameters are the same as those used in the LB simulation [20]: the same pathe pressure ratio $P_i/P_o = 2$, and $L/H = 100$. The profiles given by DSMC, IP, LB, and the slip Navier-Stokes equation are all positive nonlinear functions when $Kn = 0.0194$, which are close each other. For $Kn = 0.388$, the IP and DSMC profiles shows a remarkable agreement (Fig.5). More importantly, they are still positive, and therefore are essentially different from the LB prediction. Further study is needed to understand this difference.

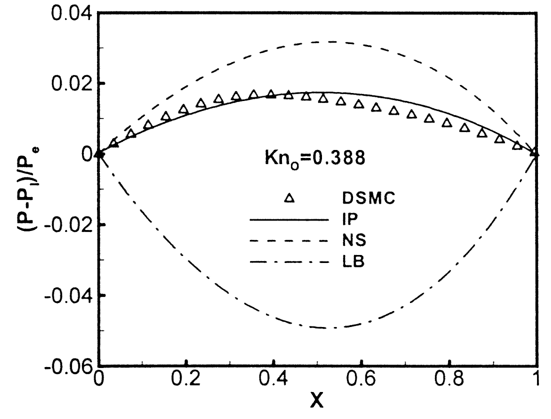


Figure 5. Comparison of streamwise pressure distributions given by DSMC, IP, slip Navier-Stokes equations with the LB solution [21].

5 DISCUSSION

In this paper we briefly review applications of the IP method in micro scale gas flows. Comparison of the velocity distributions, surface pressures and shear stresses, and mass fluxes given by IP with exact solutions at the continuum and free molecular regimes, and with the numerical solutions of the linearized Boltzmann equation [15], DSMC results, and experimental data [16-19] in the transition regime showed that IP was generally and efficiently valid for micro scale gas flows over the entire flow regime.

Because of the space limitation, some important results are not shown here, e.g. those of Sun et al [10,11]. In IP simulation of low subsonic airflows past a micro flat plate [10], the calculated drag coefficient compared well with experimental data of Schaff & Sherman [22], and Janour [23]. Introducing an additional energy transfer model to update the information temperature, Sun and Boyd [11] successfully solved the thermal Couette flows over the entire Knudsen regime. The latter demonstrated the potential of the IP method in simulating micro scale heat transfer.

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