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EXAMINATION OF THE LBM IN SIMULATION OF MICROCHANNEL FLOW IN TRANSITIONAL REGIME

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The gas flows in micro-electro-mechanical systems possess relatively large Knudsen number and usually belong to the slip flow and transitional flow regimes. Recently the lattice Boltzmann method (LBM) was proposed by Nie et al. in* Journal of Statistical Physics*, vol. 107, pp. 279–289, in 2002 to simulate the microchannel and microcavity flows in the transitional flow regime. The present article intends to test the feasibility of doing so. The results of using the lattice Boltzmann method and the direct simulation Monte Carlo method show good agreement between them for small Kn (Kn = 0.0194), poor agreement for Kn = 0.194, and large deviation for Kn = 0.388 in simulating microchannel flows. This suggests that the present version of the lattice Boltzmann method is not feasible to simulate the transitional channel flow.

Keywords lattice Boltzmann equation (LBM), microchannel flow, transitional flow regime, DSMC method

INTRODUCTION

The end of 20th century marks the beginning of the manufacture of micro-electro-mechanical systems (MEMS) and the study of the flows in them [1]. These are complicated systems manufactured by micromachining technique, including microchannels, micropumps, micronozzles, microvalves, micromotors, etc. The gas flows in MEMS, owing to their small size, possess relatively large Knudsen number $\mathrm{Kn} = \lambda/L$, where λ is the mean free path of the molecules and L is the characteristic length of the flow domain, and usually fall into the slip flow regime and the transitional flow regime. The application of the methods of molecular gas dynamics or rarefied gas dynamics is inevitable. Except in micro spacecraft applications, the gas flows in MEMS are typically of low speed, i.e., of order of several cm/s or of m/s (see, e.g., [1, 2]). The other feature of the microchannel flow is the large aspect ratio (the ratio of the channel length to height). For example, in the experiments measuring the pressure distribution [2, 3] the channels' dimensions are 1.2 μm $\times$ 30 μm $\times$ 3000 μm and 1.2 μm $\times$ 40 μm $\times$ 4000 μm, respectively. The low macroscopic speed causes the large noise-to-useful information ratio, which demands very large sampling size in statistical methods of simulation. And also, because of the low speed, the boundary value problem of the channel flow is of the elliptic nature and the

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NOMENCLATURE

a	constant in definition of mean free path
$\boldsymbol{c}_i$	particle velocities in LBM, m/s
f	distribution function
f_i	distribution function with velocity $\boldsymbol{c}_i$
h	the height of the microchannel, m
i	indicates the directions of the moving velocities along the links between the lattice notes
Kn	Knudsen number, λ/h
l	the length of the microchannel, m
$\dot{M}$	flow rate across the channel, kg/s
p	pressure, N/m^2
p_e	pressure at the exit of the channel, N/m^2
p_i	pressure at the inlet of the channel, N/m^2
p_l	linear distribution pressure, $p_l = p_e + (p_i - p_e)(1 - X)$
$\boldsymbol{r}$	particle spatial location
t	time, s
u	velocity along the axis of the channel, m/s
$\boldsymbol{u}$	velocity, m/s
$U_{\max}$	maximum velocity of the cross section, m/s
x	the Cartesian coordinate along the channel axis, m
X	dimensionless coordinate along the channel axis, $X = x/l$

Greek Symbols

α, β	indicates the spatial directions in Cartesian coordinates
δt	time step, s
λ	mean free path of the molecules, m
ρ	density, kg/m^3
τ	relaxation factor in the BGK model equation
τ'	modified relaxation factor

velocity and pressure (or density) at the inlet and exit must be regulated in dependence of each other. The large aspect ratio makes this regulation very difficult, especially for the direct simulation calculations. Recently, the lattice Boltzmann method (LBM, see [4] and reference cited therein) has been proposed and appeared as an effective numerical method for simulating fluid flows. An attempt has been made to expand this method to simulate flows with Knudsen numbers in the transitional regime [5]. This work had been done earlier [6] and some results had been presented by Karniadakis and Beskok [7]. The rarefied gas dynamics community has great interest concerning whether LBM could really be used to simulate MEMS flows in transitional regime. The purpose of the present article is to test the feasibility of LBM for transitional regime. Some results of using LBM to calculate the gas flows in microchannel obtained in [5] and in this article are compared with the direct simulation Monte Carlo (DSMC) method [8] and also with the information preservation (IP) method [9–11]. In the following section the tools in the simulation of MEMS flows have been reviewed. Next the version of LBM proposed in [5] is briefly described. Then the computation results of Nie et al. [5] (and also in this article) for the flow rates, the velocity profiles at the channel exit, and the pressure distributions along the channel are presented and compared with the DSMC (and IP) calculations. Finally, some discussion and conclusions are given.

TOOLS IN SIMULATING MEMS GAS FLOWS

In the arsenal for simulating slow rarefied gas flows there are the methods using Navier–Stokes equations with slip boundary conditions, the linearized Boltzmann equation method, the direct simulation Monte Carlo (DSMC) method, the information preservation (IP) method, and the lattice Boltzmann method, and so forth.

By its nature the Navier–Stokes equation with slip boundary conditions is appropriate only for small Knudsen number (Kn < 0.1). Recently, Kardiadakis and Beskok [7] proposed a unified flow model based on velocity scaling law for transitional flow providing results for pipe flows in agreement with the DSMC and linearized Boltzmann results, but it could not serve as a general method in the transitional regime.

The linearized Boltzmann equation method (see, e.g., [12, 13]) is suitable for solving the low-speed rarefied gas flows and its solutions for benchmark problems may serve for criteria of testing other methods. But most existing solutions are limited to simple geometry. The solution of the BGK equation [14] is much simpler, but to make it match with physical reality some correction must be made, and there are small discrepancies between the BGK and real molecule model solutions [15, 16].

The DSMC method [8] is an appropriate means to treat the rarefied gas flow in MEMS; its performance in giving global and microscopic characteristics for rarefied flow has been verified by experimental results [17, 18]. The converged DSMC simulation can be used to test the validity of other methods. But the useful information of the DSMC is drowned by huge background noise when simulating low-speed gas flows in MEMS. The task of regulating the boundary conditions at the inlet and the outlet of the long channels seems as though it cannot be accomplished; currently, only simulations of high-speed or short channel flows can be seen in the literature. This method is used to test the validity of the LBM calculation, as the example chosen does not have such a large aspect ratio (100:1) and DSMC can yield convergent results with sufficient sample size.

The information preservation (IP) method [9, 10] is a method embedded in DSMC method and preserves the information of the collective behavior of an enormous number of molecules that a simulated molecule represents and the convergence time is shortened immensely. In the simulation of Couette, Poiseuille, and Rayleigh flows [9, 10] and the long channel flows [11, 19, 20] the IP method has been verified by the linearized Boltzmann and DSMC results and available experimental investigations [2, 3, 21], respectively. The IP results for the flow case considered here are also presented for comparison.

The lattice Boltzmann method (see [4] and references cited therein) solves the simplified Boltzmann equation on lattice points. LBM solution converges to the Navier–Stokes solution for small Kn. The ease of LBM in handling complex geometry, simplicity in implementation, and its high efficiency makes it tempting to use in simulating gas flows in MEMS. Recently Nie et al. [5] attempted to use it in transitional regime and their results were reported earlier [6] and also by Karniadakis and Beskok [7]. It is of fervent concern to know whether LBM could be used to simulate transitional regime flows in MEMS. The purpose of the present article is to test the feasibility of LBM in simulating transitional flows by comparing its results with the DSMC simulation.

THE RECENT VERSION OF LBM FOR SIMULATION OF FLUID FLOW

In the following, the recent version of the LBM by Nie et al. [5] is introduced briefly (for a more detailed account see [5]). The relaxation parameter τ in the lattice Boltzmann equation with BGK collision approximation is modified as

$$\tau' = \frac{1}{2} + \frac{1}{\rho}\left(\tau - \frac{1}{2}\right) \tag{1}$$

which guarantees the constancy of the dynamic viscosity μ, and the kinematic viscosity ν is expressed as

$$\nu = c_s^2(2\tau - 1)/2\rho \tag{2}$$

where ρ is the density and c_s is the sound speed of the gas. The mean free path λ is defined as

$$\lambda = a(\tau - 0.5)/\rho \tag{3}$$

where a is constant and is chosen to be 0.388 to match the simulation results and experimental data for flow rates. So the Knudsen number can be expressed as

$$\mathrm{Kn} = \frac{a(\tau - 0.5)}{\rho h} \tag{4}$$

where h is the characteristic length of the flow.

In the calculation of the channel flow in [5] and in the present article the so-called D2Q9 lattice model [22] is used. The lattice Boltzmann BGK equation is written as

$$f_i(\boldsymbol{r} + c_i\delta t, t + \delta t) - f_i(\boldsymbol{r}, t) = -\frac{f_i - f_i^{eq}}{\tau} \tag{5}$$

The equilibrium distribution [22] is taken as

$$f_i^{eq} = t_i\rho\left[1 + \frac{c_{i\alpha}u_\alpha}{c_s^2} + \frac{(c_{i\alpha}c_{i\beta} - c_s^2\delta_{\alpha\beta})}{2c_s^4}u_\alpha u_\beta\right] \tag{6}$$

where $c_s = 1/\sqrt{3}$, $t_0 = 4/9$, $t_i = 1/9$ for $i = 1, 2, 3, 4$, $t_i = 1/36$ for $i = 5, 6, 7, 8$, α and β denote the Cartesian directions, and the fluid density ρ and velocity $\boldsymbol{u}$ are defined as

$$\rho = \sum_i f_i, \qquad \rho\boldsymbol{u} = \sum_i \boldsymbol{c}_i f_i \tag{7}$$

The bounce-back scheme is used as the boundary condition at the solid wall: when a particle reaches a lattice node in a layer adjacent to and inside the wall it scatters back to the fluid nodes along its incoming direction. The extrapolation scheme suggested in Chen et al. [23] is used at the inlet and the exit of the channel and serves as the pressure boundary condition. The density at the inlet and the exit is always kept as ρ_i and ρ_e determined from the pressure condition, and the extrapolation scheme regulates the pressure distribution among the lattice nodes between the inlet and exit of the channel, an evolution process takes place and converges to an established state when the flow rate at each cross section of the channel has the same value.

The present article follows strictly this version of LBM and only adds a couple of calculation examples to compare with the calculation by the DSMC method.

COMPUTATION RESULTS AND COMPARISON

The numerical example studied by LBM in Nie et al. [5] and in the present article is the gas flow in a two-dimensional microchannel with length l and height h. The pressure at the inlet is p_i and at the exit is p_e. The length to height ratio l/h is taken to be 100, and the pressure ratio p_i/p_e of 2 and 1.4 is imposed in the simulations. Various rarefaction cases of Kn = 0.0194, Kn = 0.194, and Kn = 0.388 have been studied. DSMC simulation is used to test the validity of the LBM results. As IP simulation results are conveniently obtained together with the DSMC results, they are also given for comparison. The results presented here of using LBM obtained by Nie et al. [5] and in the present article include the flow rate $\dot{M}$ at various Knudsen numbers, the velocity profile $u/U_{\max}$ at the exit of the channel normalized by the maximum velocity $U_{\max}$ (which changes with Kn from simulation to simulation) and the deviation $(p - p_l)/p_e$ of the pressure distribution from the linear distributed pressure $p_l = p_e + (p_i - p_e)(1 - X)$ (with $X = x/l$ where x is the coordinate in the axial direction).

The flow rate $\dot{M}$ as a function of Kn obtained by different methods are shown in Figure 1. The results of LBM for Kn = 0.0194 and 0.194 are in agreement with those of other methods. The flow rate for Kn = 0.388 by LBM is higher than predicted by other methods. On the whole, the prediction of LBM for the flow rate is good, and this is understandable, for the constant a in Eq. (3) has been determined from the best match of the simulation mass rate with experiments [5].

The velocity profile and the pressure distribution results are presented for Kn = 0.0194, 0.194, and 0.388 in Figures 2 to 7, respectively. For Kn = 0.0194 the flow is in the slip flow regime, and the velocity profile at the channel exit and the pressure distribution obtained by LBM are in good agreement with the results of DSMC, IP, and slip Navier–Stokes calculations (Figs. 2 and 3 show the results for a pressure ratio of $p_i/p_e = 1.4$). Figure 3 shows certain difference between the LBM and DSMC (and IP)

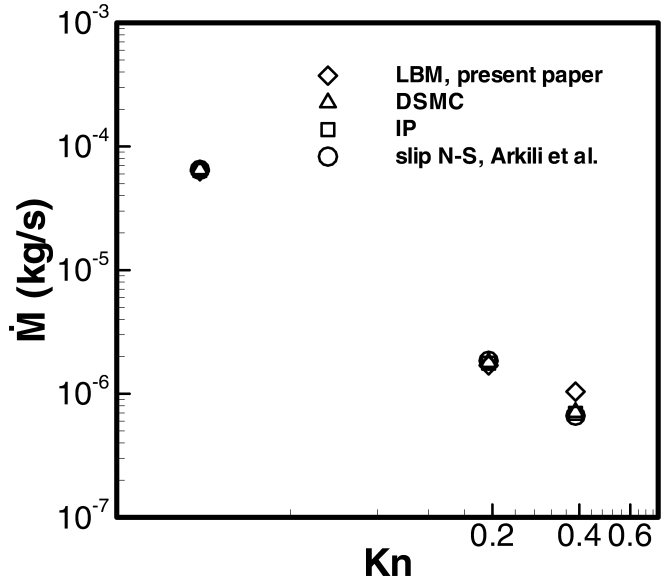

Figure 1. The variation of mass flow rates with the exit Knudsen numbers.

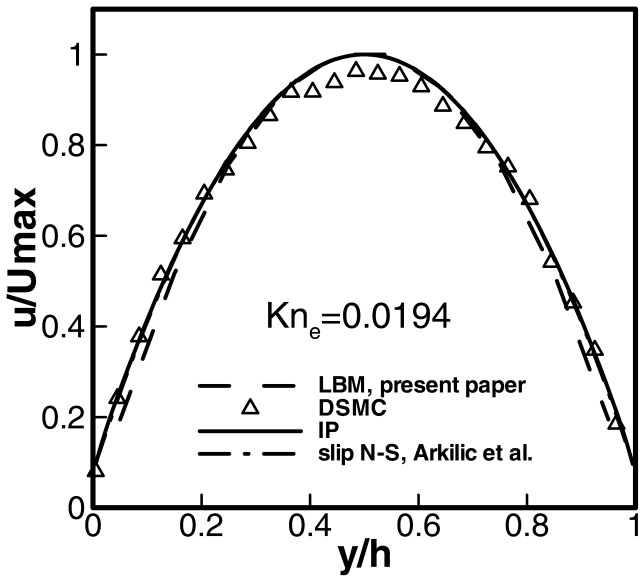

Figure 2. Velocity profiles at the channel exit. Comparison of LBM, DSMC, and IP simulations, Kn $= 0.0194$, $p_i/p_e = 1.4$.

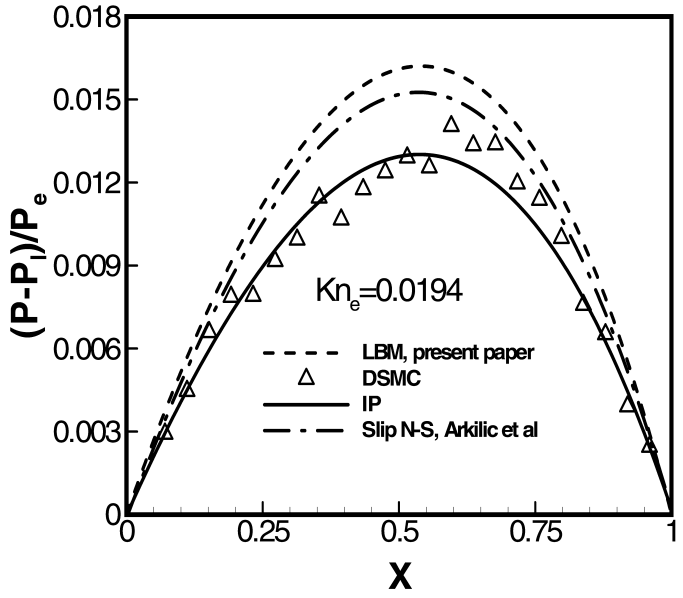

Figure 3. Deviation of pressure distribution from linearity. Comparison of LBM, DSMC, and IP simulations, Kn $= 0.0194$, $p_i/p_e = 1.4$.

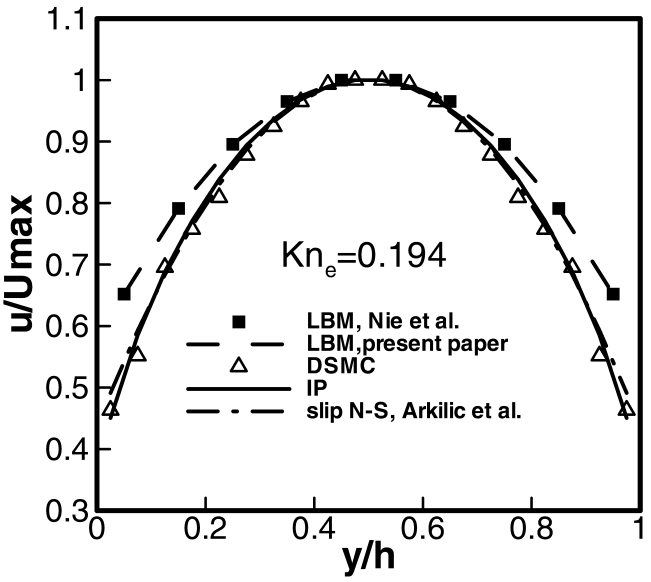

Figure 4. Velocity profiles at the channel exit. Comparison of LBM, DSMC, and IP simulations, Kn = 0.194, $p_i/p_e = 2.0$.

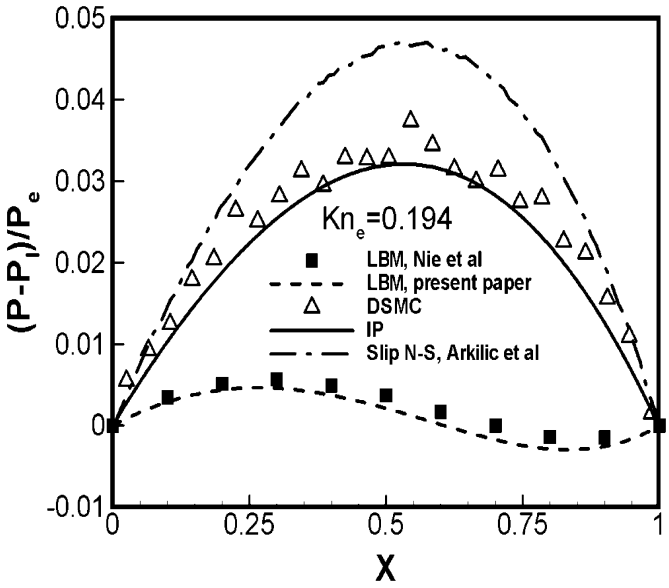

Figure 5. Deviation of pressure distribution from linearity. Comparison of LBM, DSMC, and IP simulations, Kn = 0.194, $p_i/p_e = 2.0$.

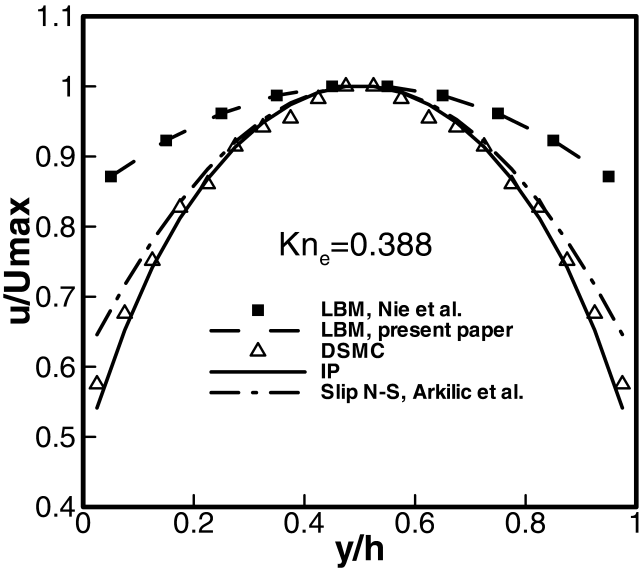

Figure 6. Velocity profiles at the channel exit. Comparison of LBM, DSMC, and IP simulations, Kn = 0.388, $p_i/p_e = 2.0$.

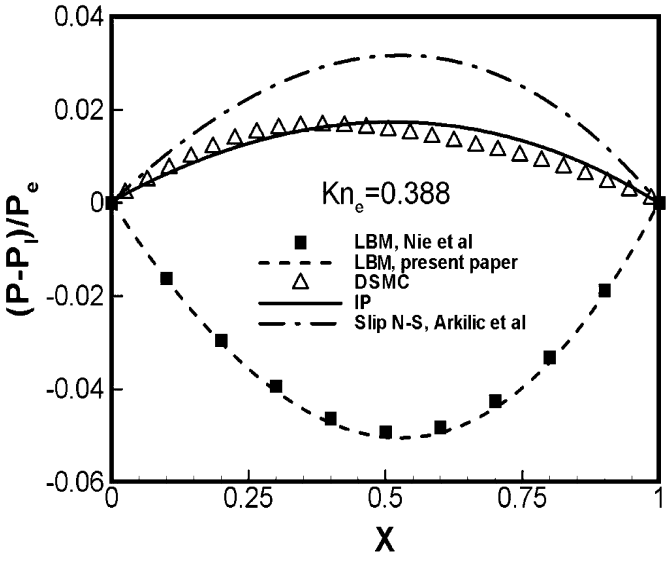

Figure 7. Deviation of pressure distribution from linearity. Comparison of LBM, DSMC, and IP simulations, Kn = 0.388, $p_i/p_e = 2.0$.

Table 1. Sample sizes used to yield the DSMC and IP data

Pressure ratio (p_i/p_e)	Knudsen number (Kn)	Sample size for DSMC	Sample size for IP
1.4	0.0194	6.6×10^6	7.4×10^4
2	0.0194	1×10^7	7.5×10^4
2	0.194	6×10^6	1.4×10^4
2	0.388	5.6×10^6	1.4×10^4

results, but this is only a small difference enlarged by the way of presentation. This verifies the feasibility of using LBM to simulate MEMS gas flows in continuum and slip flow regime for small Kn.

For Kn = 0.194 the velocity profile at the exit obtained by LBM shows certain minor difference from those obtained by all other three methods (see Fig. 4, with $p_i/p_e = 2$). More apparent is the difference in the deviation from linear pressure distribution in the case of Kn = 0.194 (see Fig. 5, with $p_i/p_e = 2$). The LBM result of $(p - p_l)/p_e$ swings closely around the null line, while the DSMC (and IP) results show clear large positive deviation from linearity.

It should be noted that the fluctuations of DSMC simulation results shown in Figures 3 and 5 are still very high, although enormous sample sizes have already been employed. The sample sizes used to yield the DSMC and IP results are listed in Table 1 and a computation time about 5 days on a Pentium-IV 1.5G PC is needed to obtain one DSMC result.

When Knudsen number increases further to Kn = 0.388, the flow falls into the transitional flow regime, the LBM velocity profile shows clear deviation from the results of DSMC and IP (Fig. 6, with $p_i/p_e = 2$), and the negative behavior of $(p - p_l)/p_e$ predicted by LBM contrasts in strong relief with the positive prediction of DSMC and IP (Fig. 7, with $p_i/p_e = 2$). This shows the unfeasibility of LBM in simulating MEMS flow in transitional flow regime.

DISCUSSIONS AND CONCLUSION

It seems very tempting to use the lattice Boltzmann method (LBM) to simulate gas flows in MEMS. The present study reveals that LBM is suitable to simulate MEMS flows only for very small Knudsen numbers, as it retains certain advantages over conventional method as easy handling of complex geometry, simplicity in implementation, and high efficiency in this near continuum regime. For Knudsen number as large as Kn = 0.2, LBM results apparently deviate from DSMC results. In the transitional flow regime, for Kn = 0.388, LBM results deviate from DSMC results significantly and predict wrong trend in the pressure deviation from linearity. It is noted that in the DSMC simulation the Kn number is ensured to be the same as used in the LBM method, so the mean free path λ (Eq. (3)) is kept equal in both LBM and DSMC calculations, but the simulated values of the collision time and the viscosity in DSMC simulation are found to be different from those of LBM calculated from Eqs. (1) and (2). The present article has used the well-tested DSMC method to show the unfeasibility of using the lattice Boltzmann method to simulate transitional flow in MEMS. But the final judgment will be given by experimental investigation, which is very desirable.

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