A01-16691

AIAA-01-0876

Particle Simulation of Micro-Scale Gas Flows

I. D. Boyd and Q. Sun
University of Michigan
Ann Arbor, MI 48109.

39th AIAA Aerospace Sciences Meeting & Exhibit
8-11 January 2001 / Reno, NV

Particle Simulation of Micro-Scale Gas Flows

Iain D. Boyd and Quanhua Sun

Department of Aerospace Engineering
University of Michigan, Ann Arbor, MI, 48109, USA

ABSTRACT

The development of particle methods to simulate flows related to micro-electro-mechanical systems is described. This effort is aimed at increasing our understanding of rarefied gas behavior to facilitate the design and optimization of micro-devices. The proposed information preservation method preserves macroscopic information of the flow as the particles move and interact with each other and the domain boundaries. The results exhibit very low levels of statistical scatter, which helps apply the method to low speed MEMS flows. In the implementation, specific consideration is needed for flows with large temperature variation.

NOMENCLATURE

C_v	specific heat at constant volume
Kn	Knudsen number
Ma	Mach number
Re	Reynolds number
N	total sample size
R	specific gas constant
T	temperature
d	distance between two plates
k	Boltzmann constant
l	variable indicating x or y
m	mass of the molecule
n	number density
p	pressure
t	time
u	velocity in x direction
v	velocity in y direction
ρ	density
σ, σ'	velocity statistical scatter

Subscripts

0	at y = 0
s	on surface
x	in x direction
y	in y direction
∞	at free stream condition

1. INTRODUCTION

The design and fabrication of micro-electro-mechanical systems (MEMS) has developed rapidly over the last several years. The size of current MEMS is in the range from a tenth of a micron to several hundred microns, which means the Knudsen number of the flows at atmospheric pressure ranges from 0.0005 to 0.5. In rarefied gas flows (Kn>0.01), it is not correct to calculate the transport terms in the Navier-Stokes equations from macro-scale flow quantities. Methods based on a kinetic formulation must therefore be applied.

One of these methods is the direct simulation Monte Carlo (DSMC) method (Bird, 1994), which models a real gas as thousands or millions of discrete computational particles. The DSMC method has had great success in simulating hypersonic flows, and some researchers have already applied it to micro-channel flows (Oh et al., 1995, Ahn et al., 1996, Xue et al., 2000). For hypersonic flows, the boundary conditions are straightforward for the DSMC method. Particles are simply removed when they cross inlet or outlet boundaries, and a certain number of particles are injected into the cells at inlet and outlet according to a Maxwellian distribution, provided the velocity, temperature and number density at these locations are known. Besides, the boundary conditions at certain locations are not necessary, because the governing equations for supersonic flows are hyperbolic equations. However, for subsonic flows, the inflow or outflow conditions must be applied to all the boundaries since the governing equations are elliptic equations. For MEMS flows, because the domain is too small to allow measurement by common velocity diagnostics, the inflow or outflow conditions may not be available. Furthermore, it is very difficult for DSMC to isolate the useful signal from the "noise" in low speed flows. The velocity statistical scatter of air at atmospheric temperature is $\sigma = \sqrt{2RT} = 410\, m/s$. If we suppose the sample processes in DSMC are totally independent from step to step, then the statistical scatter in the final result will be $\sigma' = \sigma/\sqrt{N}$. Then the ratio of noise to signal is about 0.4 with a sample size of 10^6 when the velocity signal is 1 m/s. However, this ratio is too large to distinguish the fine structure of the flow. In order to

reduce the statistical scatter, the total sample size must be greatly increased. Hence, few flows of practical interest can be simulated due to the limit of CPU time (Oh, et al. 1995).

An alternative approach is the information preservation (IP) method (Fan and Shen, 1998), which is very effective in reducing the statistical scatter. The IP method preserves macroscopic information as the particles simulated in DSMC move and interact with each other and the domain boundaries. Recently, a 2D IP code was implemented and several cases were tested for low speed flows (Cai, et al, 1999). However, the isothermal assumption was used in the code, which limits the application of the IP method.

The main objective of the present investigation is to present the further development of the information preservation method. In section 2, the basic idea and the implementation of the IP method is described. The method has advantages for low speed flows, but it is a challenge to use the method for flows with large temperature variation. In section 3, two flows are considered to exhibit the advantages and disadvantages of the IP method. Some conclusions are given in section 4.

2. THE INFORMATION PRESERVATION METHOD

2.1 BASIC IDEA

It is generally assumed that each particle simulated in the DSMC method represents an enormous number (10^8-10^{25}) of real molecules, and the particles possess random thermal properties according to certain distribution functions. At the same time, those real molecules must have certain aggregate information. In this meaning, the particle simulated in DSMC carries the aggregate information and the statistical scatter as a whole. The information preservation method aims to preserve the aggregate information of the real molecules. The information (momentum and energy) preserved in the IP method changes when the particles move and interact with each other and the boundaries. However, the information is conserved even for rarefied gas flows, except that care must be taken with viscosity and thermal conductivity. These effects can be considered during the particle collisions and gas-surface interactions. Then two steps at each time level are considered: the Lagrangian step and the Eulerian step. During the Lagrangian step, the information of particles that are selected to collide is adjusted according to general conservation laws. When particles cross edges or reflect from a wall, certain information transfer may happen. During the Eulerian step, the preserved information is updated according to the Euler equations. At the end of each time level, the cell information is sampled since it is needed by the next time step. Figure 1 illustrates the whole procedure for the IP method.

2.2 IMPLEMENTATION

In principle, any microscopic information of the flow can be preserved by the simulated particles. For MEMS gas flows, non-equilibrium between the translational energy and internal energy is not significant. In our 2D parallel code that is based

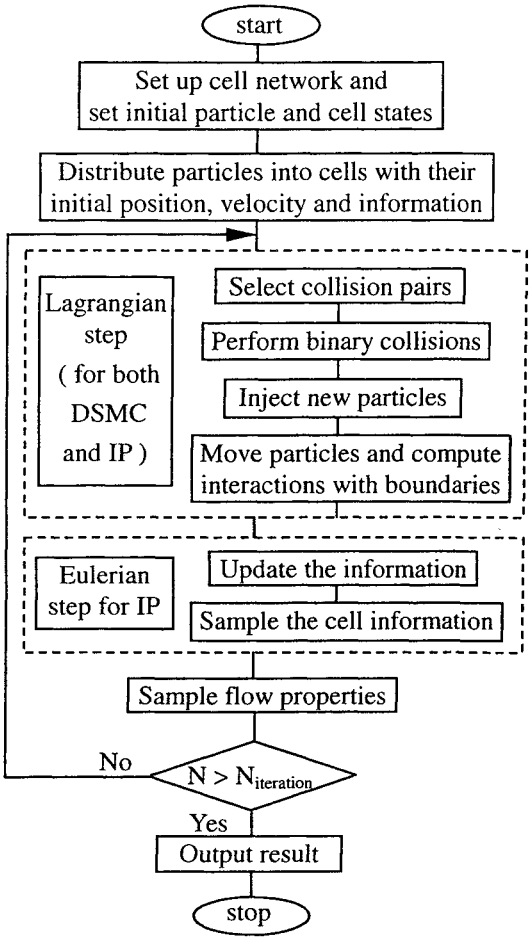


Figure 1. DSMC-IP flowchart

on a parallel optimized DSMC code named "MONACO" (Dietrich and Boyd, 1996), number density, velocity in two-dimensions, and translational temperatures in three-dimensions are preserved.

The information for all the particles and cells is initialized by the ambient condition. If new particles are injected into the computational domain, the ambient condition or the local cell information is given to the new particles according to the boundary conditions. For binary collisions, the momentum and energy conservation laws are used. It is assumed that the preserved velocity and preserved temperatures of two particles are the same after the collision. When a particle collides with a wall, the information of the particle is changed. If it is a specular reflection, the preserved temperatures of the particle are kept unchanged and the preserved velocity component of the particle perpendicular to the wall is reversed. If it is a fully diffuse reflection, the preserved temperatures of the particle are accommodated to the wall temperature and the preserved velocity of the particle is set to the velocity of the wall.

The 2D Euler equations can be expressed as follows:

$$\frac{d\rho}{dt} = -\frac{1}{\rho}\left[\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right] \tag{1}$$

$$\frac{du}{dt} = -\frac{1}{\rho}\frac{\partial p}{\partial x} \tag{2}$$

$$\frac{dv}{dt} = -\frac{1}{\rho}\frac{\partial p}{\partial y} \tag{3}$$

$$\frac{d\left[C_v \cdot T + \frac{u^2+v^2}{2}\right]}{dt} = -\frac{1}{\rho}\frac{\partial [pu]}{\partial x} - \frac{1}{\rho}\frac{\partial [pv]}{\partial y} \tag{4}$$

Here, $\frac{d}{dt}$ is the full derivative and $\frac{\partial}{\partial t}$ is the partial derivative. In 2D non-equilibrium flows, these equations are modified as:

$$\frac{d[1/n]}{dt} = \frac{1}{n}\left[\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right] \tag{5}$$

$$\frac{du}{dt} = -\frac{1}{n \cdot m}\frac{\partial p_x}{\partial x} \tag{6}$$

$$\frac{dv}{dt} = -\frac{1}{n \cdot m}\frac{\partial p_y}{\partial y} \tag{7}$$

$$\frac{d\left[\frac{1}{2}R \cdot T_x + \frac{u^2}{2}\right]}{dt} = -\frac{1}{n \cdot m}\frac{\partial [p_x \cdot u]}{\partial x} \tag{8}$$

$$\frac{d\left[\frac{1}{2}R \cdot T_y + \frac{v^2}{2}\right]}{dt} = -\frac{1}{n \cdot m}\frac{\partial [p_y \cdot v]}{\partial y} \tag{9}$$

where $\frac{\partial}{\partial l} = \frac{\oiint_{cell} \frac{\partial}{\partial l} dxdy}{\oiint_{cell} 1 \cdot dxdy}$, $l = x$ or y (10)

However, it is difficult to calculate the derivatives because only the information of discrete particles is preserved. The derivatives on the right hand side are calculated from the cell values sampled from the particles. If n on the right hand side is replaced by the ratio of the real number of particles in the cell to the volume of the cell, the conservation properties can still be guaranteed. Notice that the concept of number density is not good for a single particle, so the number density of a particle takes the value of the number density for the cell at the end of each time step.

2.3 ADVANTAGES AND DISADVANTAGES

The IP method preserves the information of the flow, which contains a much smaller level of statistical scatter compared with the DSMC method for MEMS flows. In DSMC, the statistical scatter comes directly from the thermal movement of particles. In IP, the thermal movement of particles causes the statistical scatter only at the information level. Hence, the statistical scatter of the information can not be larger than the variation of the information in the whole flow field. For MEMS flow at atmospheric temperature with the characteristic speed of 1 m/s, the velocity statistical scatter in IP is less than 1 m/s, while it is 410 m/s in DSMC. Hence, the IP method can greatly reduce the computational cost for low speed flows. The simulation of many practical MEMS flows becomes possible. The IP method also helps apply boundary conditions for the DSMC method, which improves the application of the DSMC method.

A disadvantage of the IP method is that it is difficult to model the translational energy flux. The energy flux through a cell edge or a wall is zero in equilibrium flows. However, for gas at rest, the average translational energy for particles crossing the edge from one side is 2kT, which is different from 3/2kT, the average translational energy for particles in the cell. This difference is important when calculating the heat flux from the wall or when the flow is a non-equilibrium flow. The difference comes because the translational energy flux of the part in the direction perpendicular to the wall or the edge is twice the flux of the part in the other directions in equilibrium flows, which is a direct result from the microscopic movement of the molecules. One possible way to include this difference in the IP method is to introduce additional translational energy flux in that direction. Notice that the translational energy flux from one side is balanced by the flux from the opposite side in equilibrium flows. The calculation of the additional energy flux is based on the difference between the temperature of the particle and the temperature of the cell in the direction perpendicular to the cell edge or the wall. The difficulty here is how to assign the additional energy to the particles.

In our implementation, when a particle crosses a cell edge, it carries its information to the new cell. Also, an additional energy of $\frac{1}{2}k(T_p - T_c)\cdot w_p$ is transferred from the original cell to the new cell. Here, T_p and T_c are the temperature of the particle and the temperature of the cell in the direction perpendicular to the cell edge, respectively, and w_p is the particle weight of the original cell. The additional energy is uniformly distributed over all particles in the cell at the end of that time step. Here, the additional energy is divided by the particle weight since each particle represents a large number of molecules. A similar treatment is applied when a particle interacts with a wall except that the additional energy of $\frac{1}{2}k(T_w - T_p)\cdot w_p$ is transferred from the wall to the cell. However, investigation shows that the translational energy flux across a cell edge or from a wall in this model is not sufficient. It may be that the treatment of the additional energy reduces the difference of the temperatures between particle and cell. Hence, the additional energy may be increased to $\frac{1}{2}k(T_p - T_c)\cdot w_p \cdot a$,

where a is greater than unity. Then further study is needed to fix the value of a. For many subsonic, micro-scale gas flows, the temperature variation is not large, and then the effect here will not be important.

3. RESULTS AND DISCUSSION

Two example flows are calculated with the information preservation method. One is the flow over a NACA 0012 airfoil, which is used to show the usefulness of the IP method. The other is the flow between two parallel plates at different temperatures, which exhibits a difficulty in the IP method.

3.1 FLOW OVER A NACA 0012 AIRFOIL

Consider air flow around a NACA 0012 airfoil with a chord length of 0.04 m. The flows are simulated under two conditions listed in Table 1, where Re_∞ and Kn_∞ are based on the chord length. Three numerical methods are compared: the DSMC method, the continuum approach with a slip boundary condition (Fan, et al, 1999) and the IP method.

Table 1. Free stream conditions

Case	Ma_∞	Re_∞	ρ_∞ (kg/m^3)	T_∞ (K)	U_∞ (m/s)	Kn_∞
A	0.8	73	1.116×10^{-4}	257	257	0.014
B	0.1	1	1.315×10^{-4}	290	34	0.013

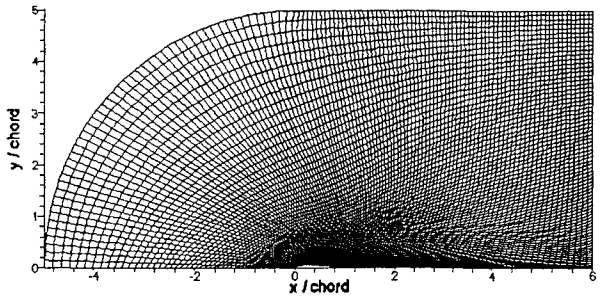
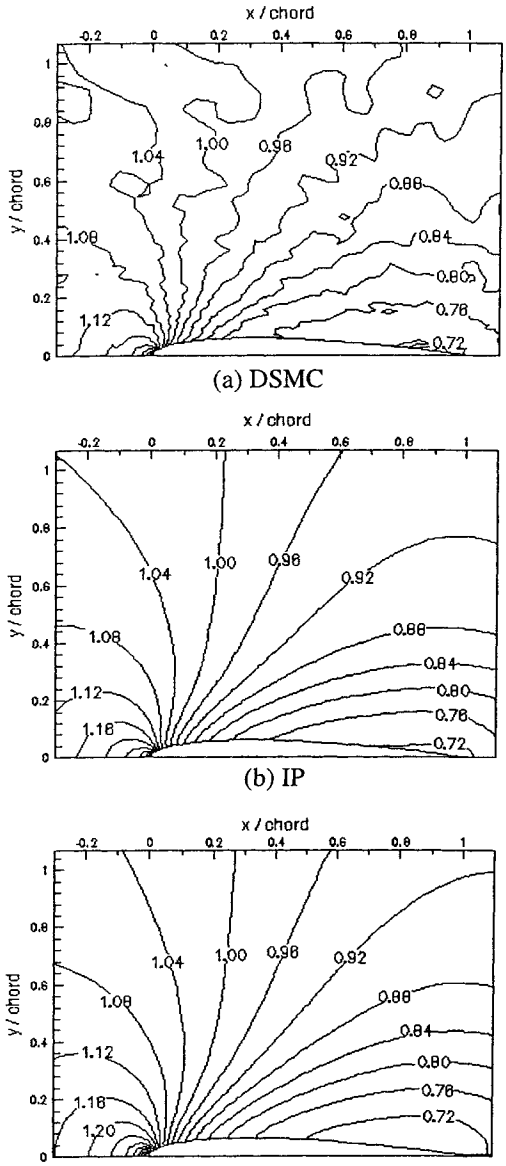


Figure 2. Computational grid for flow over a NACA 0012 airfoil

The computational domain is shown in Fig. 2, which has considered the symmetry of the problem. The whole domain is divided into 9120 non-uniform structured cells that are clustered to the airfoil. On average, about 45 particles in case A and 40 particles in case B are located in each cell. Free stream flow conditions are applied to all the boundaries except for the symmetric line of the airfoil, since the computation domain is much larger than the airfoil. The time step is set to 5×10^{-8} s, which is smaller than the mean collision time of particles. In order to reach the steady state, 30,000 iterations are executed before sampling the flow field.

Figure 3 shows the density contours non-dimensionalized by the free stream density for case A. The total sample size used in the DSMC results and the IP results is about 450,000 particles per cell. However, the contours in the DSMC results



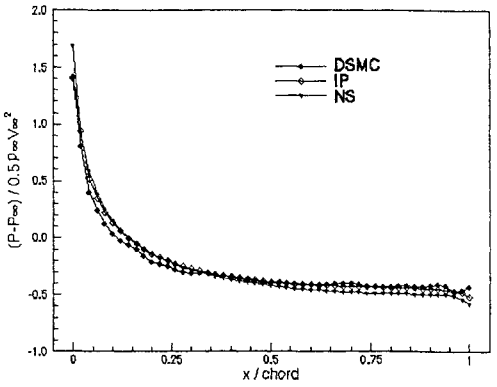
(a) DSMC

(b) IP

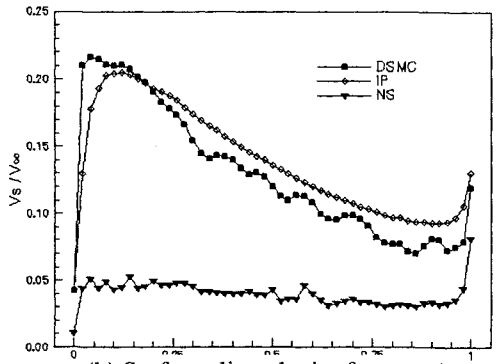
(c) Continuum approach with a slip boundary condition

Figure 3. Comparison of density flow fields for case A

are still not smooth because of the statistical scatter. The simulated density distribution exhibits the same basic features in the three methods. Good agreement between the DSMC results and the IP results are obtained except for a small difference near the leading edge. However, this difference between the DSMC results (Fig. 3a) and the IP results (Fig. 3b) is smaller than the difference between the DSMC results (Fig. 3a) and the results from the continuum approach with a slip boundary condition (Fig. 3c). A comparison of the pressure and slip velocity on the airfoil surface among the three methods is shown in Fig. 4. The three methods predict very similar pressure distributions on the surface (Fig. 4a), but give different slip velocity distributions (Fig. 4b). The continuum approach



(a) Surface pressure for case A

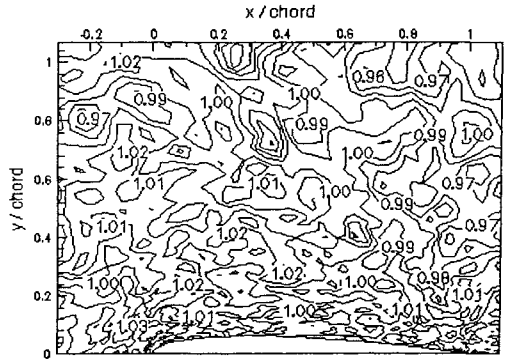


(b) Surface slip velocity for case A

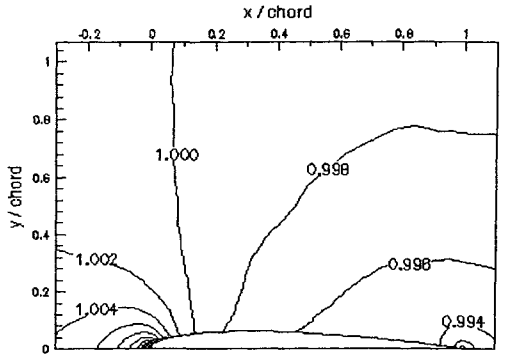
Figure 4. Comparison of surface properties for case A

predicts much smaller slip velocities than the other two methods that are relatively close to each other. This may indicate that the Navier-Stokes equations in the continuum approach are invalid for a small region around the airfoil. Further investigation is needed to address this problem. In this case, the IP method predicts similar results to the DSMC method, which illustrates the utility of the information preservation method.

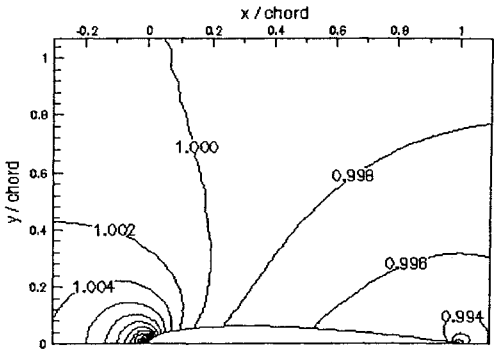
Figure 5 shows the density contours non-dimensionalized by the free stream density for case B. When the total sampling size is about 400,000 particles per cell, reasonable results are obtained by the IP method (Fig. 5b), while the large scatter in the DSMC method makes it impossible to obtain meaningful results (Fig. 5a). Clearly, the IP method is able to simulate low speed flows. Comparison is also made between the IP results (Fig. 5b) and the results from the continuum approach with a slip boundary condition (Fig 5c). The density contours are very similar. The difference near the leading edge is similar to that in case A, in which the continuum approach predicts a higher density than the IP method. Figure 6 shows a comparison of the pressure and slip velocity on the airfoil surface between the IP results and the results from the continuum approach. As in case A, both methods give similar pressure distributions on the surface (Fig. 6a), and the continuum approach predicts a smaller slip velocity than the IP method (Fig. 6b).



(a) DSMC



(b) IP

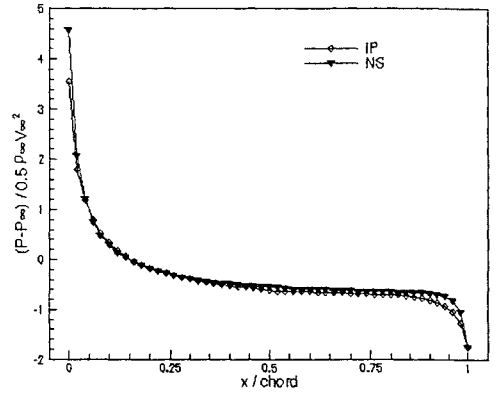


(c) Continuum approach with a slip boundary condition

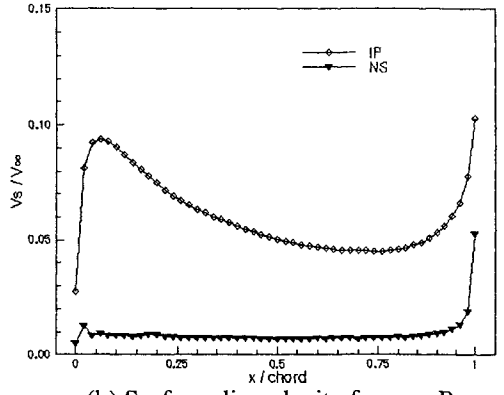
Figure 5. Comparison of density flow fields for case B

3.2 FLOW BETWEEN TWO PLATES AT DIFFERENT TEMPERATURES

Flow between two plates at different temperatures has been studied experimentally for different Knudsen numbers. The Knudsen number is defined as the ratio of the mean free path of the molecules located at the centerline to the distance between the plates. Figure 7 shows the geometry used in the experiment (Teagan and Springer, 1968). The distance between two 25.4-cm-long plates was 2.5 cm. This is therefore approximately a one-dimensional problem. The temperature of the lower plate was kept at 288 K, while the upper plate was at 368 K. The argon gas between the plates was at a steady state condition during the experiment. The thermal accommodation coefficient



(a) Surface pressure for case B



(b) Surface slip velocity for case B

Figure 6. Comparison of surface properties for case B

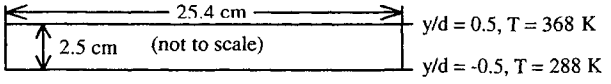


Figure 7. Parallel plate geometry

was evaluated to be 0.826 using data obtained in the free-molecular regime.

In the simulation, 99 cells equally divide the whole regime between the plates (300 cells are used when Kn = 0.01). Thus, the cell size is less than the mean free path of particles. A total of 60,000 to 90,000 particles are simulated for all the cases. The time step is 1×10^{-7} s, which is smaller than the mean collision time for all cases. The results are obtained by sampling 2,000 time steps after the code is run for 20,000 time steps, which assumes a steady state is reached.

Figure 8 compares the simulated density from the IP method with the experimental data. When the Knudsen number is 0.01, it is found that the IP results agree well with the DSMC results (not shown). It is clear that the agreement between the IP results and the experimental data decreases as the Knudsen number increases. This is because the model of the energy flux across the cell moves the flow towards equilibrium. Thus the IP

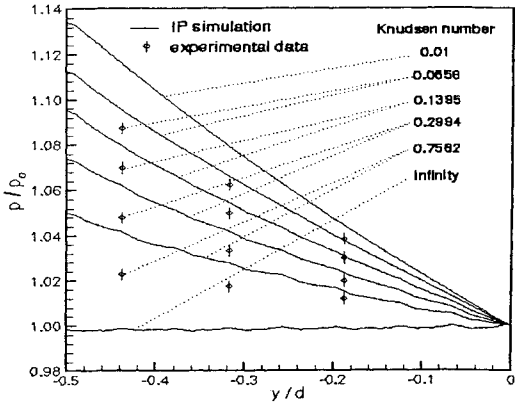


Figure 8. Density profiles

result is close to the experimental data at a certain smaller Knudsen number. However, good agreement between the IP results and the theoretical solutions (uniform field) is obtained when the flow becomes free-molecular. Figure 9 compares the IP results with the continuum solution and the experimental data at y/d = -0.4375. In comparison to the continuum solution, the IP results agree with the experimental data in an engineering context.

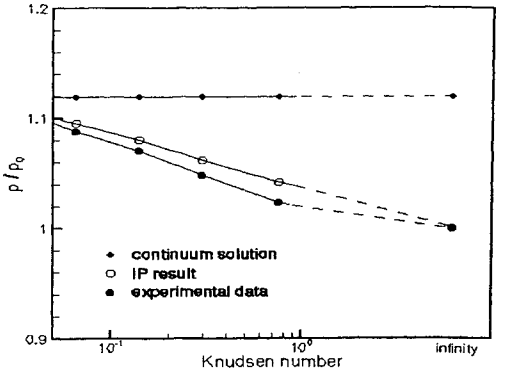


Figure 9. Density comparison at y/d = -0.4375

An endeavor is made to account for the effect in the energy flux model of the IP method that occurs because the additional energy is equally shared by the particles. It is expected that additional energy flux is required to reduce this effect. Figure 10 shows the density distribution for several energy flux adjustments when the Knudsen number is 0.2994. It is clear that increasing the energy flux can counter balance the effect to some degree. Investigation also finds that the energy flux adjustment depends on the local Knudsen number. Less energy flux adjustment is needed when the Knudsen number is higher. In Fig. 10, notice that excess energy flux is introduced near the wall since the local Knudsen number is very high. Clearly, further work is required to formulate a physically accurate energy flux model for the IP method.

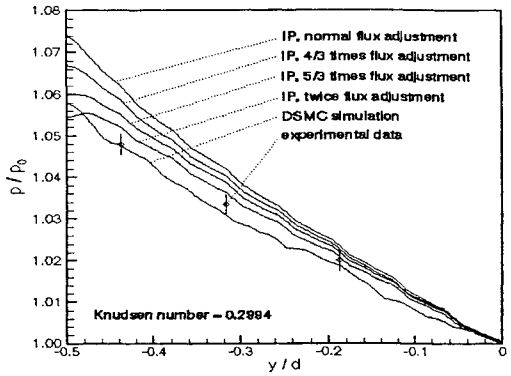


Figure 10. Density distribution with energy flux adjustment

4. CONCLUSIONS

MEMS gas flows are in general rarefied gas flows. The DSMC method can be used for this type of flow. However, large statistical scatter limits the application of the DSMC method when the speed of the flows is slow. In this paper, the information preservation method was further developed for two-dimensional MEMS gas flows.

The simulation results showed that the IP method worked effectively for the flows over a NACA 0012 airfoil. It greatly reduced the statistical scatter, which enables the application of particle methods.

A difficulty was encountered in modeling energy flux in the IP method. Specific consideration was needed for flows with large temperature variation. In our implementation, additional energy flux was introduced when simulated particles crossed the cells and interacted with the boundaries. In comparison to a continuum solution, the IP results were much closer to the experimental data.

ACKNOWLEDGMENTS

The authors thank Dr. G. V. Candler of the University of Minnesota for providing the Navier-Stokes results for the flow over the NACA 0012 airfoil. This work was supported by the Air Force Office of Scientific Research through MURI grant F49620-98-1-0433.

REFERENCES

Ahn, J.C., Mavriplis, C., and Goulard, R, "Heat Transfer and Flow Fields in Microchannels Using the DSMC Simulation Method," AIAA, 96-0361, 1996

Bird, G.A., *"Molecular Gas Dynamics and the Direct Simulation of Gas Flows,"* Clarendon, 1994

Cai, C.P., Boyd, I.D., Fan, J. and Candler, G.V., "Direct Simulation Method for Low-speed Micro-Channel-Flows," AIAA, 99-3801, 1999

Dietrich, S., and Boyd, I.D., "Scalar and Parallel Optimized Implementation of the Direct Simulation Monte Carlo Method", *Journal of Computational Physics*, Volume 126, pp. 328-342, 1996

Fan, J., and Shen, C., "Statistical Simulation of Low-Speed Unidirectional flows in Transition Regime," in *Proceedings of the 21th International Symposium on Rarefied Gas Dynamics*, edited by R. Brum, et al., Marseille, 1998, pp. 245-252

Fan, J., Boyd, I.D., Cai, C.P., Hennighausen, K. and Candler, G.V., "Computation of Rarefied gas flows around a NACA 0012 Airfoil," AIAA, 99-3804, 1999

Ho, C.M., and Tai, Y.C., "Micro-Electro-Mechanical-Systems (MEMS) and Fluid Flows," *Annual Review of Fluid Mechanics*, Volume 30, pp. 579-612, 1998

Nance, R.P., Hash, D.B., and Hassan, H.A., "Role of Boundary Conditions in Monte Carlo Simulation of MEMS Devices," *Journal of Thermophysics and Heat Transfer*, Volume 12, Number 3, pp. 447-449, 1998

Oh, C.K., Oran E.S., and Cybyk, B.Z., "Microchannel Flow Computed with the DSMG-MLG," AIAA, 95-2090, 1995

Ohwada, T., "Heat Flow and Temperature and Density Distribution in a Rarefied Gas between Parallel Plates with Different Temperatures. Finite-Difference Analysis of the Nonlinear Boltzmann Equation for Hard-sphere Molecules," *Physics of Fluids*, Volume 8, Number 8, pp. 2153-2160, 1996

Piekos, E.S., and Breuer, K.S., "DSMC Modeling of Micromechanical Devices," AIAA, 95-2089, 1995

Teagan, W.P., and Springer, G.S., "Heat-Transfer and Density-Distribution Measurements between parallel Plates in the Transition Regime," *The Physics of Fluids*, Volume 11, Number 3, pp. 497-506, 1968

Xue, H., Fan, Q. and Shu, C., "Prediction of Micro-Channel Flows Using Direct Simulation Monte Carlo," *Probabilistic Engineering Mechanics,* Volume 15, pp. 213-219, 2000