Efficient DSMC Modeling Techniques for Micro/Nano Gas Flows

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ABSTRACT

Gas flows encountered in micro/nano scale devices are often low speed and non-continuum. The Direct Simulation Monte Carlo (DSMC), a popular molecular based simulation technique for rarefied gas, has proven to be inefficient in dealing with low-speed gas flows. In this paper, we present the Octant Flux Splitting Information Preserving DSMC (OSIP-DSMC) method as an efficient DSMC method for micro/nano gas flows, particularly those driven by thermal loading. The efficiency of the proposed method has been demonstrated through several examples including thermal transpiration.
Keywords: rarefied gas flows, thermally driven micro/nano gas flows, DSMC, thermal transpiration

1 INTRODUCTION

At small scale, gas flows behave very differently from their macro counterparts. It is possible to move gas molecules simply by creating a thermal gradient inside the gas. One such example is the thermal transpiration in which a pressure gradient is established inside a micro channel as a result of the creep flows caused by the applied thermal gradient. Such a principle has been utilized in building Knudsen's compressors and creating on-chip vacuum environment for MEMS devices [1,2]. The unique behavior of micro/nano gas flows opens many doors for the development of new micro devices and instruments. This in turn calls for the development of modeling techniques and tools to increase our fundamental understanding of gas behavior and to assist in the design of these micro devices.

Modeling of micro/nano gas flows is challenged by their (1) non-continuum effects and (2) low speed. The non-continuum effects require molecular modeling approaches. A common molecular simulation method suitable for rarefied gas is the Direct Simulation Monte Carlo (DSMC) [3]. Initially developed for modeling high-speed, high-altitude gas dynamics, the DSMC has achieved a great success in a variety of applications. However, when applied to the modeling of micro/nano gas flows with typical velocities less than 10 m/s, a great number of samples must be taken in order to control the inherent statistical noise to an acceptable level. For example, for a gas flow with a stream velocity on the order of 1 m/s, about 8×10^6 independent samples are required to achieve 1% resolution. This prohibits the application of the DSMC in realistic MEMS problems.

The slow convergence of the DSMC simulations of low-speed flows has motivated the development of several specialized DSMC techniques such as those proposed by Pan, et al. [4,5] . A promising technique, the information preserving DSMC (IP-DSMC) [6,7,8], seeks to reduce noise by preserving collective quantities of each simulation molecule and macroscopic quantities are obtained by averaging the collective instead of the microscopic information of each molecule. Successful applications of the IP-DSMC have been demonstrated on several benchmark problems, particularly those without temperature variation. We found, however, for certain non-isothermal problems such as thermal transpiration, the existing IP-DSMC methods have failed to produce a correct flow pattern set up by the thermal gradient.

In this paper, we report our recently developed technique, the Octant-Flux-Splitting Information Preserving DSMC technique (OSIP-DSMC), for the modeling of low-speed, non-isothermal rarefied gas flows. A brief description of the method is present next. It is followed by the results of two sample problems: thermal transpiration and thermal cavity. A summary of the finding is given in section 4.

2 THE OSIP-DSMC TECHNIQUE

The DSMC is a stochastic molecular dynamics simulation method in which each simulation molecule is a statistical representation of a large cluster of real molecules. These molecules move according to their microscopic velocities and interact with each other following a probabilistic treatment of collision. Macroscopic quantities are obtained by averaging the microscopic quantities of each simulation molecule. In the OSIP-DSMC, in addition to microscopic quantities, the information-preserving (IP) velocity and temperature, denoted as $\mathbf{V}$ and T_{IP}, are initially assigned and subsequently updated for each simulation molecule. These quantities can be regarded as the collective information of the real molecules that each simulation molecule represents. They are transported along with each molecule and are modified after each collision either with wall or with each other. The update of the IP quantities is determined by the following transport

equations. These equations are derived based on conservation laws.

$$\frac{\partial(nm)}{\partial t} + \nabla \cdot \left(nm\bar{\mathbf{V}} \right) = 0 \ , \qquad (1)$$

$$\frac{\partial\left(nm\bar{\mathbf{V}} \right)}{\partial t} + \nabla \cdot \left(nm\overline{\mathbf{cV}} \right) = -\nabla \cdot \left(nm\overline{\mathbf{c}'\mathbf{c}'''} \right), \qquad (2)$$

$$\frac{\partial}{\partial t}\left(nm\left(\overline{V^2} + 3\mathrm{R}T_{IP}\right)\right) + \nabla \cdot \left(nm\overline{\mathbf{c}\left(V^2 + 3\mathrm{R}T_{IP}\right)}\right) = -\nabla \cdot \left(nm\overline{\mathbf{c}'\left(V^2 + 3\mathrm{R}T_{IP} - c^2\right)}\right) \qquad (3)$$

In these equations, n is the number density, m is the molecular mass, $\mathbf{c}$ is the molecular velocity, $\mathbf{c}' = \mathbf{c} - \mathbf{c}_0$ is the peculiar velocity, $c_0 = \bar{\mathbf{c}} = \bar{\mathbf{V}}$ is the stream velocity, and $\mathbf{c}''' = \mathbf{c} - \mathbf{V}$. The second terms on the left hand side of Eqs. 2 and 3 are convective terms, corresponding to the changes in the IP quantities due to microscopic movement of simulation molecules. The right-hand sides in Equations 2 and 3 are the pseudo force and heat flux terms resulting from the gradient of the stress tensor and energy.

A crucial step in the OSIP-DSMC method is the evaluation of the pseudo force and heat flux, i.e., the right-hand sides of Eqs. 2 and 3. They are calculated by assuming the velocity density function of each simulation molecule is a Maxwell-Boltzmann distribution, but with a bias velocity space. Based on the direction of its velocity, each molecule is classified as belonging to only one octant of the whole velocity space. By integrating the density function with stress tensor or energy over the corresponding velocity space, the pseudo force and heat flux are evaluated for each simulation molecule. This approach captures the modality in velocity distribution function caused by non-equilibrium sources such as thermal gradient, while the previous methods fail to do so.

In summary, the main steps in the OSIP-DSMC are listed as follows.

1. Determine the local coordinate system from the local heat flux vector, **q** and construct the transformation matrix, **R** composed of column vectors defining the local coordinate system.
2. Perform a coordinate transformation on the stream velocity, splitting velocity, and the individual microscopic and IP velocities.
3. Calculate the pseudo force and heat flux for each simulation molecule and average over the molecules in each splitting direction. Sum the contributions from each splitting direction to obtain the complete correlation coefficients
4. Return the correlation coefficients to the global coordinate system,
5. Proceed with Modification step of IP-DSMC (Eqs (1)-(3)) and sample steps.

3 RESULTS

We present two examples in this section: thermal transpiration and thermal cavity flow. In both cases, results obtained from the OSIP-DSMC method are compared with those from the DSMC. In the thermal-transpiration example, semi-analytical results obtained from the solution of a linearized Boltzmann Transport equation are also presented.

3.1 Thermal Transpiration

The problem considered is a sealed 2-D microchannel with a rectangular cross section with a length of 5 μm and a height of 1 μm. The two ends of the channel are maintained at two different temperatures with a linear temperature gradient along the length of the channel and T_1 = 273 K and T_2 = 573 K and the working gas (Argon) is initially at a uniform pressure $P(x,y) = P = 1$ atm. The walls are considered to be fully accommodating and the height is much larger than the width, allowing the simplification to two dimensions.

The OSIP-DSMC simulation (and underlying DSMC) was allowed to run for 60,000 timesteps prior to beginning sampling. The simulations then proceeded for and additional 288,000 timesteps accumulating 24,000 samples. The temperature profiles within the gas in both the DSMC and OSIP-DSMC simulations follow the linear temperature distribution imposed by the boundary conditions (see Figures 1 and 2). The DSMC simulation predicts a static pressure gradient as shown in Fig. 3. However, unlike the previous methods, the Octant Splitting method also predicts a static pressure gradient (see Fig. 4). The magnitudes of the OSIP-DSMC pressure gradient varies from 100.447 kPa to 103.239 kPa, which compares well with the DSMC pressure gradient of 100.110 kPa to 103.688 kPa.

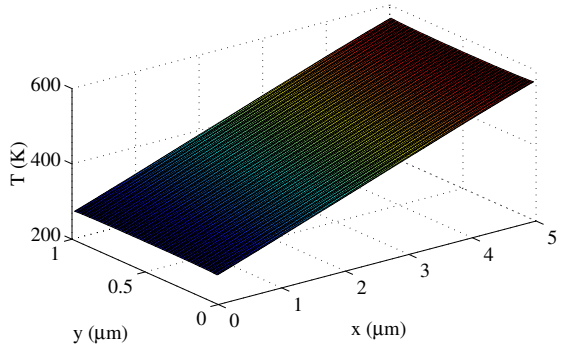

Figure 1. DSMC temperature.

(1)

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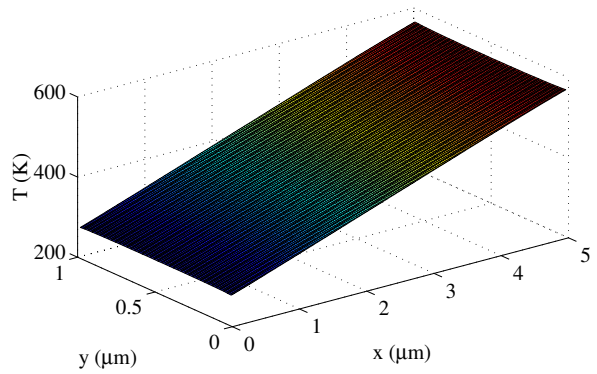

Figure 2. OSIP-DSMC temperature.

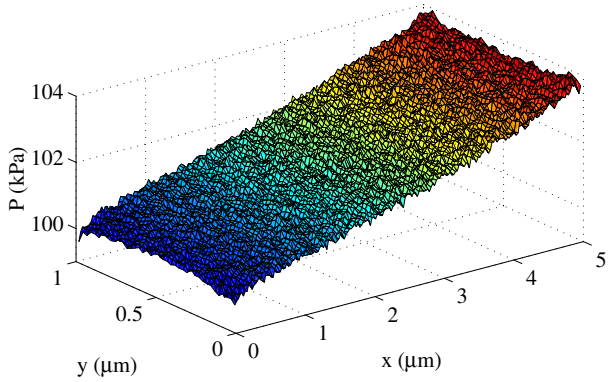

Figure 3. DSMC pressure.

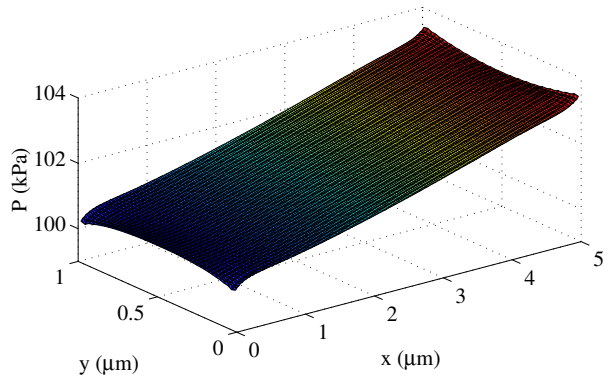

Figure 4. OSIP-DSMC pressure.

The velocity fields are presented Figures 5 and 6. While both plots exhibit the expected recirculatory flow patteren, the significant reduction in noise is clearly visible in the OSIP-DSMC result. To achieve the resolution obtained by the OSIP-DSMC, the DSMC would require significantly more samples. The maximum velocity observed in the OSIP-DSMC is 0.872 m/s and occurs near the wall.

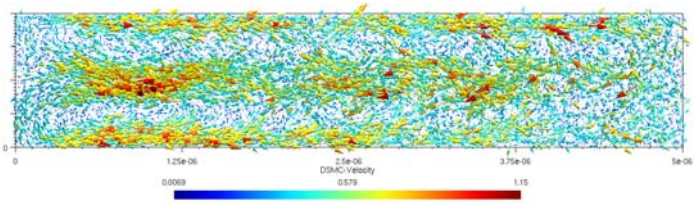

Figure 5. DSMC velocity field.

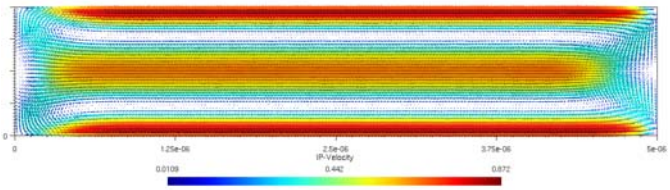

Figure 6. OSIP-DSMC velocity field.

Additional simulations were performed for thermal transpiration systems subject to the same loading, but with channel widths of 100 nm and 20 nm. The pressure profiles for these, as well as the 1 μm wide channel are presented in Fig. 7. As an additional point of comparison, the linearized BTE solution for the thermal transpiration problem proposed by Sharipov [9] is included. Considering the different modeling techniques and the obvious noise remaining in the DSMC results, the correspondence between the three models is quite good and demonstrates the ability of the OSIP-DSMC to provide detailed information of all flow characteristics at a substantially lower computational expense than the DSMC.

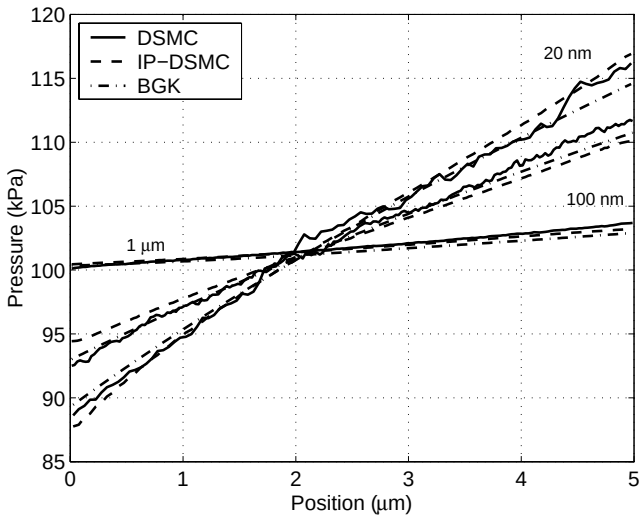

Figure 7. Pressure for different channel heights, (DSMC, OSIP-DSMC, Sharipov).

3.2 Thermal Cavity Problem

As another illustration, gas inside a sealed 2-D domain ($1\mu m \times 1\mu m$) with one wall maintained at a temperature of *400 K* and the others maintained at a temperature of *200 K* was simulated. Due to symmetry, only half of the domain was discretized with 40 cells in the x-direction and 20 in the y-direction. The cells are initialized with an average of 100 particles per cell and an initial uniform pressure of 1 atm (corresponding to Kn ≈ 0.1). The results of the DSMC and OSIP-DSMC simulations are presented in Figures 8 and 9, respectively. The simulation was stopped after 12,000 samples. While the DSMC is far from convergence, the flow is fully resolved in the OSIP-DSMC simulation and demonstrates a recirculatory flow with a maximum velocity of approximately 0.5 m/s.

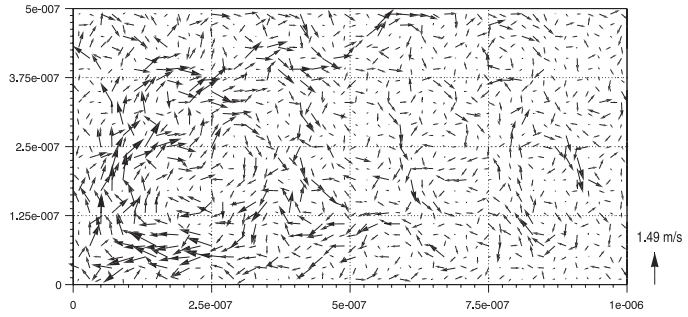

Figure 8. DSMC velocity field.

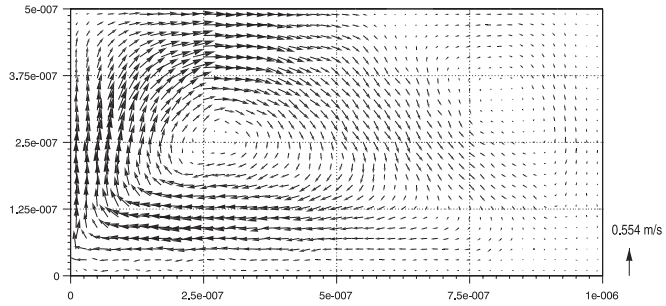

Figure 9. OSIP-DSMC velocity field.

4 SUMMARY

For modeling of low-speed, non-equilibrium rarefied gas flows, an efficient molecular simulation method, the Octant-Flux-Splitting IP-DSMC method, has been developed. By properly preserving the collective information of each simulation molecule, the statistical noise inherent in the original DSMC is greatly reduced, resulting in a much smaller set of required samples. The efficiency and accuracy of the method have been demonstrated through two model problems: thermal transpiration and thermal cavity flow by comparing the OSIP-DSMC solutions with the DSMC and the linearized BTE solutions. Although further validation is needed, the OSIP-DSMC method has shown its promise in becoming an efficient and accurate method for modeling realistic MEMS/NEMS gas flow problems.

REFERENCES

[1] S. E. Vargo, E. P. Muntz, G. R. Shiflett, and W. C. Tang, "Knudsen Compressor as a Micro- and Macroscale Vacuum Pump Without Moving Parts or Fluids," *Journal of Vacuum Science and Technology A*, vol. 17, pp. 2308-2313, 1999.

[2] S. McNamara and Y. B. Gianchandani, "On-Chip Vacuum Generated by a Micromachined Knudsen Pump," *Journal of Microelectromechanical Systems*, vol. 14, pp. 741- 746, 2005.

[3] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*: Clarendon Press ; Oxford University Press, 1994.

[4] L. S. Pan, G. R. Liu, B. C. Khoo, and B. Song, "A Modified Direct Simulation Monte Carlo Method for Low-Speed Microflows," *Journal of Micromechanics and Microengineering*, vol. 10, pp. 21-27, 2000.

[5] L. S. Pan, T. Y. Ng, D. Xu, and K. Y. Lam, "Molecular Block Model Direct Simulation Monte Carlo Method for Low Velocity Microgas Flows," *Journal of Micromechanics and Microengineering*, vol. 11, pp. 181-188, 2001.

[6] J. Fan and C. Shen, "Statistical Simulation of Low-Speed Rarefied Gas Flows," *Journal of Computational Physics*, vol. 167, pp. 393-412, 2001.

[7] Q. Sun and I. D. Boyd, "A Direct Simulation Method for Subsonic Microscale Gas Flows," *Journal of Computational Physics*, vol. 179, pp. 400-425, 2002.

[8] Q. Sun and I. D. Boyd, "Theoretical Development of the Information Preserving Method for Strongly Nonequilibrium Gas Flows," presented at 38th AIAA Thermophysics Conference, Toronto, Ontario, Canada, 2005.

[9] F. Sharipov, "Non-isothermal Gas Flow Through Rectangular Microchannels," *Journal of Micromechanics and Microengineering*, vol. 9, pp. 394-401, 1999.