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DECREASING STATISTICAL NOISE IN THERMAL CREEP FLOWS

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Abstract

In DSMC method flow velocities are sampled using the average of the individual molecular velocities. Consequently, solution of creeping flows by DSMC method requires an enormous number of samplings because of the high ratio between molecular and flow velocities. In this study a new method is proposed to calculate flow velocities with the help of mass flux rates instead of individual molecular velocities. For this reason a thermally driven cavity flow is composed as a test problem. Following, this test problem is solved using both a slightly modified DSMC method and a conventional DSMC method. Mass flux rate and conventional models produce similar results in terms of flow velocities. But statistical error is not minimized as expected. It is concluded not only the mass flux but also the momentum and heat fluxes should also be incorporated into the future studies to reduce statistical errors in creeping flows.

Key words: Thermal creep, DSMC, cavity flows, rarefied gas

INTRODUCTION

In this study a two-dimensional rarefied gas flow in a square cavity is investigated. This flow is induced by linear temperature gradients on both upper and lower walls. In rarefied gas conditions, the mean-free-path (λ) which is the average distance between consecutive molecule collisions is comparable with characteristic length (L) of the flow geometry. Actually, the ratio of the mean-free-path and characteristic length (L) is known as Knudsen number (Kn) which is dimensionless.

$$Kn = \frac{\lambda}{L}. \tag{1}$$

Generally, *Kn* is used to measure the degree of rarefaction of gases. If *Kn* is lower than the 0.01, continuum based solvers are used to calculate the flow properties. In some cases, such as low gas density or small characteristic length (L), *Kn* can become higher than the 0.01. In these rarefied flow regimes, because of the inadequate molecular collisions, flow departs from the local equilibrium and conventional constitutive equations lose their validity. Continuum based solvers requires new type of non-linear constitutive equations. These new equations are called Burnett equations. These equations are very difficult to solve because of the complicated boundary conditions and stability problems. In high *Kn* regimes, molecular based solvers supersede the continuum based ones. Direct simulation Monte Carlo (DSMC) is one of these methods **(Bird, 1994)**. This stochastic particle method has shown produce conformal results with the experimental studies. The first disadvantage of this method is the

computational load in low *Kn* regimes. But new techniques are developed and the application range of the DSMC method continues extending into the lower *Kn* number regimes **(Bird, 2009)**. One other problem with the DSMC method is the slow convergence in the creeping flows, because of the statistical noise (**Chen, 2001**). As a gas kinetic theory based method, all the macroscopic properties are calculated from the microscopic properties in DSMC method. The order of magnitude between molecular speeds of the gas molecules and flow velocities of the creeping flows is more than two. To calculate the slow flow velocities, the statistical noise in the DSMC method should be at least two orders of magnitude lower than the flow velocity. As an example, to simulate 1 m/s gas flow at standard temperature and pressure within 1% error, $8x10^6$ samples are required **(Masters and Ye, 2007)**. This tremendous number of sampling can be intolerable in terms of the computation time.

To increase the efficiency of the DSMC method in slow creeping flows, new techniques are developed. At the beginning, studies are intensified on the molecular velocities. It is aimed that, separating the random (thermal) and flow velocities from each other, statistical error can be reduced with less sampling. In information preservation (IP) DSMC method, instead of changing the DSMC method considerably, small additions are made without changing the main character of the DSMC method **(Fan and Shen, 1998)**. Here only the new information velocities which are collective velocities of the enormous number of molecules represented by the DSMC molecules are attached to the DSMC molecules. Following IP-DSMC method is further developed to be implemented to more benchmark problems **(Cai et al., 2000)**. Although this method is successful in isothermal flows, new approaches are needed for non-isothermal flows such as thermally driven cavity flows. Two new models are proposed to use IP-DSMC method in non-isothermal flows **(Sun and Boyd, 2002, Sun and Boyd, 2005).** Although these IP-DSMC methods are shown successfully for some benchmark problems such as Poiseuille and Couette flows, they are still not satisfactory for the thermally creeping flows. As a result a new model based on the IP-DSMC method is developed to analyze thermally driven cavity flows **(Masters and Ye, 2007)**. This new method is called "Octant" flux splitting IP-DSMC (OSIP-DSMC). Aside from the IP-DSMC method, some other models are also proposed to decrease the statistical error of the DSMC method with less sampling. In order to reduce the statistical error, a low "artificial temperature" concept is put forward and relation between thermodynamic temperature and kinetic energy of the gas molecules are inquired **(Pan et al., 2000)**. But this model only works with isothermal flows. In molecular block model **(Pan et al., 2001)**, conventional DSMC molecules are replaced with a heavier and different cross section molecules to reduce the sampling number for both isothermal and non-isothermal slow gas flows. But this method is shown as not accurate **(Wang and Li, 2004)**. Later, a new method is proposed using both "ghost" and "real" molecules together in DSMC simulations **(Chun and Koch, 2005)**. Here the DSMC method is modified, using a variable weighting of particles during both collision and sampling steps. In this method the number of "ghost" molecules can escalate exponentially with time unless *Kn* is high. Additional measures are needed to prevent the model become unstable. This method is only validated with two simple models and needed to be further improved. Moreover some trials are done to filter out the statistical noise coming from the conventional DSMC method in lower velocities **(Kaplan and Oran, 2000)**. But more work is needed to validate this method especially in low Mach numbers. Finally, low-variance (LV) DSMC method is developed to overcome these difficulties and limitations **(Radtke et al., 2011)**. It is claimed that by incorporating mass conservation into the LVDSMC model, 10 particles per cell is enough to obtain accurate results in transition regime. But further studies are required to investigate the convergence behavior of this methodology in terms of the time step (Δt) and cell dimension (Δx).

Here a new point of view is put forward in order to decrease the statistical error of the DSMC method when low velocity gas flows are in question. It is known that these statistical errors are stemmed from the order of magnitude difference between the thermal $(\mathbf{c}')$ and the mean $(\bar{\mathbf{c}})$ molecule velocities. First, a possibility is investigated if mean velocity can be correctly calculated from the mass flow rate $(\dot{m})$ between DSMC cell surfmoleculartead of total molecule velocities $(\mathbf{c})$ as in the current DSMC solvers. Secondly, it is aimed that the existing DSMC solver is only slightly modified. So with the exception of flow velocities all other macroscopic properties such as pressure, temperature and density are still calculated as in the conventional DSMC method.

DSMC METHOD

DSMC method is a simplified version of the molecular dynamics (MD) method. To reduce the computational load each DSMC molecule represents many physical molecules. Additionally molecule movements and collisions are decoupled. The DSMC method consists of four main steps **(Bird, 1994)**. In the first step all the DSMC molecules in the flow geometry change their positions according to the velocities they own. This step is called " movement" step. In the "indexing" step, all the DSMC molecules indexed to the DSMC cells according to their positions. The third step is "collision" step. In this step DSMC molecules collide with the partner molecules based on models taken from the kinetic theory. Finally, in the last phase called "sampling" step, macroscopic properties like pressure, temperature, density and flow velocities are calculated using microscopic properties. These microscopic properties are only limited to the positions and the velocities of the DSMC molecules.

In this study it is planned only to change the calculation method of the flow velocities in the "sampling" step. Current DSMC solvers use individual velocities $(c_{i,n})$ of the DSMC molecules positioned in the same cells to calculate the flow velocities $(\overline{c_i})$ as shown below,

$$\overline{c_i} = \frac{1}{N}\sum_{n=1}^{N} c_{i,n}. \tag{2}$$

N presents the total number of DSMC molecules in this cell. Although this technique produces correct results in all velocity ranges, sampling numbers can be intolerable when the flow speed is much lower than the thermal velocities of the molecules. In this proposed model, flow velocities are calculated from the mass flow rates $(\dot{m})$ between DSMC cell surfaces. Mass flow rates for a 2D flow geometry are shown in Fig.1 in both x- and y- directions.

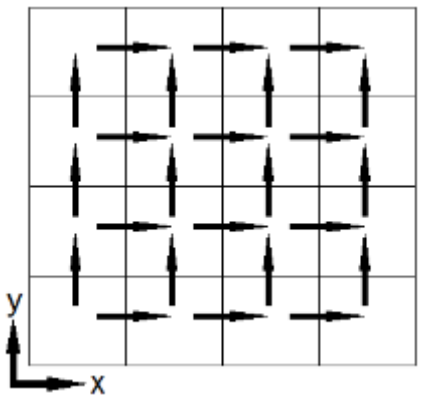

Fig.1. Mass flows between DSMC cell surfaces in a 2D flow geometry

Because of the decoupling of the molecule movements and collisions, DSMC cell dimensions (Δx) and time steps (Δt) are scaled with mean-free-path (λ) and local collision time (Δt_c) respectively. If DSMC cell sizes are chosen larger than the mean-free-path, enhanced transport coefficients are developed (**Karniadakis and Beskok, 2002**). DSMC molecules travel more than one cell without a collision chance if large time steps (Δt) are employed. Again this kind of deficiency results with incorrect transport coefficients (**Karniadakis and Beskok, 2002**). In this study, to avoid the incorrect transport coefficients, cell sizes and time step are restricted by the limitations stated above. As a result, the probability of a DSMC molecule travel more than one cell is highly unlikely. Each DSMC molecule is traced during "movement" step to calculate the mass flow rates on the cell surfaces. In this technique, each cell surface passed through the DSMC molecule is recorded starting from the first molecule to the last molecule. Because of the time step limitation, only the 24 cells around the departure cell are taken into account as shown in Fig.2..

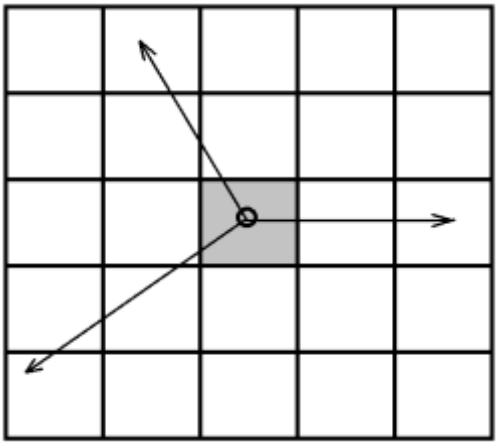

Fig.2. DSMC molecule travels among cells through the cell surfaces

Each molecule adds a mass flow rate $(\dot{m})$ to the cell surface according to the Equation stated below,

$$\dot{m} = \frac{\dot{N}\, m\, F_N}{\Delta t}. \tag{3}$$

The number of the molecules passes through the surface in one time step, molecule mass and the number of the real molecules represented by the one DSMC molecule are $\dot{N}$, m and F_N respectively. The mass flow rate can also be stated by macroscopic properties as,

$$\dot{m} = \rho\, A U. \tag{4}$$

Here density, surface area and flow velocity are presented by ρ, A and U respectively. Merging both (3) and (4), a new relation to the flow velocity on the cell surface is derived,

$$U = \frac{\dot{N}\, m\, F_N}{\rho\, A\, \Delta t}. \tag{5}$$

To calculate the velocity components on the DSMC cell centers, it is assumed that the averages of the two velocities on both cell surfaces are equal to the velocities on the cell centers for all DSMC cells.

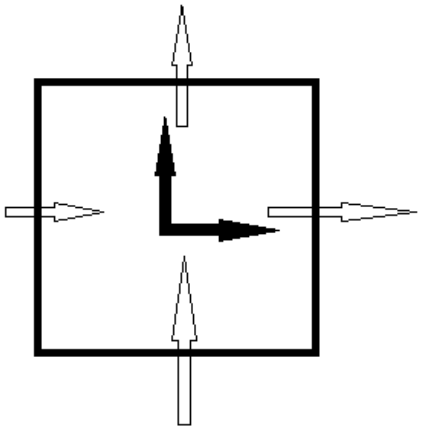

Fig.3. Cell velocities derived from the surface velocities

RESULTS

In order to validate the assumptions and proposed new model, a test problem is solved with both conventional and modified DSMC solver. The dimensions of the square cavity are $L=2x10^{-6}$ m in both directions. There is a linear temperature gradient on both upper and lower walls. The temperatures of the left and right walls are 400^0 K and 600^0 K. Argon is used as working gas in this simulation. Knudsen number is calculated as 0.2 for this simulation. Consequently, gas flow is in transition regime. Test problem is shown in Fig.4.

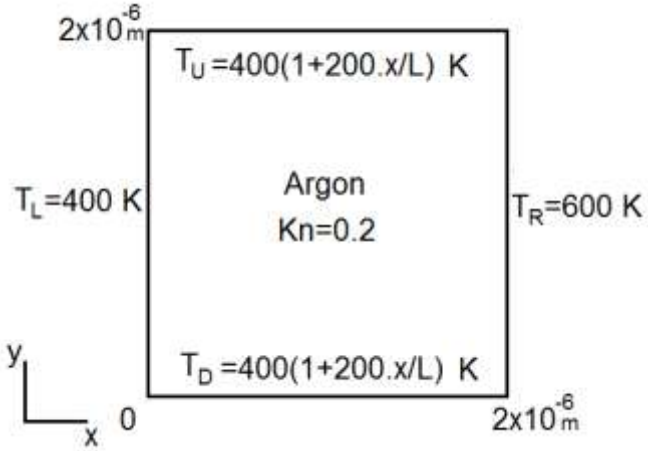

Fig.4. Test problem

Variable hard sphere (VHS) model is used in collision simulations. Wall-molecule collisions are modeled with fully diffuse reflections with complete thermal accommodation. Because of the symmetry in y-direction, simulation is carried out only one-half of the flow geometry. A total of 55 DSMC cells and 2508 DSMC molecules are used. The results are summoned in Fig.5.

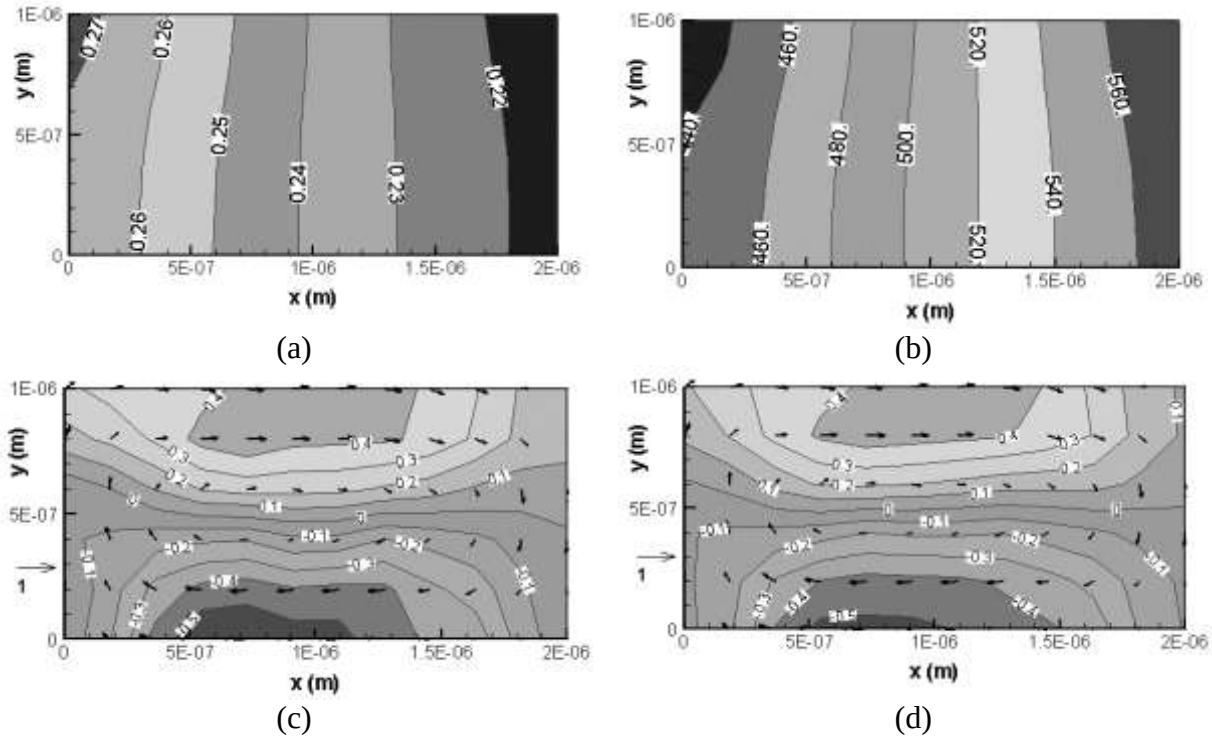

Fig.5. DSMC simulation results for the thermally driven creeping flow in a square cavity, (a) Density contours (kg/m^3) (b) Temperature contours (K) (c) Velocity component (m/s) in x-direction calculated with conventional method (d) Velocity component (m/s) in x-direction calculated with mass flux rate method

These results are obtained after 500000 time steps. Statistical noise levels both in density and temperature contour values are quite low. But in flow velocity contours, statistical noise is still quite high in the conventional model. In case of the mass flux rate method, similar results are derived compare to the conventional model. But an improvement in terms of the statistical noise is not occurring.

CONCLUSIONS

To sum up, analyzing creeping gas flows with DSMC method is computationally quite expensive. Although many methods are put forward to solve this deficiency, none of these are flawless. In this study, DSMC method is slightly modified to calculate the flow velocities of the gas flow with the help of mass flow rates instead of molecular velocities. At the same time it is also aimed to reduce statistical error stemmed from the high ratio between the thermal velocities of the DSMC molecules and slow flow velocities. Although the new proposed method is successful to calculate the flow velocities using mass flow rates, statistical error is not minimized as expected. It is evaluated that, solving creeping flows with a DSMC method with less statistical error is a more fundamental problem than it is anticipated. Consequently, when dealing with statistical noise in creeping flows, not only the mass flux but also the heat and momentum fluxes should be taken into account. Future studies will definitely build on the mass flux rates, but at the same time these additional issues will also be incorporated into the investigations.

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