Analysis of Internal Micro-Scale Gas Flows with Pressure Boundaries Using The DSMC Method

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ABSTRACT. The development and applications of a two-dimensional DSMC (Direct Simulation Monte Carlo) program for pressure boundaries using unstructured cells and its applications to typical internal micro-scale gas flows, including a micro-manifold, a micro-nozzle and a slider air bearing of computer hard disk, are described. This is aimed to further test the treatment of pressure boundaries by particle flux conservation, especially at subsonic speed, to gas flows involving many exits, more complicated geometry and moving boundaries. Firstly, results of a T-shaped micro-manifold with inlet Knudsen number of 0.2 show that excellent mass flow conservation between the inlet and two exits is obtained at low subsonic gas flows. Secondly, a micro-nozzle with the fixed inlet Knudsen number of 0.067 is simulated. For higher specified pressure ratio (exit to inlet), the location of maximum Mach number moves further downstream as the pressure ratio decreases; while, for lower specified pressure ratio, the Mach number increases all the way through the nozzle to the exit. Eventually, supersonic speed is observed at the exit for pressure ratio equal to or less than 0.143. Thirdly, for the gas flows of a slider air bearing of computer hard drive, the results agree very well with those of Alexander et al. (Phys. Fluids, 1994) for all the simulated conditions. In summary, the particle flux conservation concept has been proved successfully at multiple (more than two) pressure boundaries with complicated geometries and moving solid boundaries.

INTRODUCTION

Micro-electro-mechanical systems (MEMS) are becoming prevalent both in commercial and industrial research due to the rapid growth and developments in the semiconductor industry. MEMS are the field with strong multi-disciplinary research needs. Applications for these devices include consumer products (e.g., airbag triggers, micro-mirror displays), industrial and medical tools (e.g., micro-valves, micro-motors), and instrumentation (e.g., micro pressure sensors, micro shear stress sensors) [1].

The shrinking size of MEMS (order of a micron) has several advantages over the corresponding macro-scale systems. First, they can be fabricated quite inexpensive and in large quantities, borrowing mature techniques developed in the semiconductor industry. Second, the miniature inertia (due to small size) allows them to respond very quickly to excitation, enabling the fabrication of actuators and sensors with frequency responses previously unimaginable for related mechanical systems [2].

In the past, most research was conducted concerning the electrical and mechanical properties of MEMS. Relatively few researches [8] focused on the thermal and fluid effects on MEMS performance, including rarefaction, thermal creep and compressibility. Hence, the understanding of these physical effects is very important for the design optimization of these very small-scale devices.

For most MEMS flows, the Knudsen numbers are generally located in the slip-flow and transitional-flow regimes due to their micro scales, even at atmospheric condition. An example of such a micro-scale device is a side-driven micro-motor [3]. The typical gap between the base and the rotor is 3 μm, the corresponding Kn equal to 0.05. Another example of large Kn is the modern Winchester-type hard disk drive mechanism, where the read/write head floats about 60 nm or less above the surface of the spinning platter [4]. The corresponding Kn is equal to 1.1. Hence, the rarefaction effects, often neglected in traditional analysis, have to be carefully considered and modeled in micro-scale gas flows.

The direct simulation Monte Carlo (DSMC) method, first introduced by Bird [5], has been recognized as a de-facto method for studying rarefied gas dynamics. It has been applied very successfully to rarefied hypersonic flows [5] and other more fundamental scientific problems, such as flow instabilities [6]. In addition to the space science
applications, it has also been utilized in the analysis of ultra-high vacuum technology [7]. Very recently, it was
applied to rarefied internal gas flow problems such as channel, pipe and duct flows and the results agree very well
with experiments [8]. Most importantly, DSMC is the only practical way to deal with flows in the transitional regime,
without resorting to the difficult Boltzmann equation, which requires modeling an integral-differential (collision)
term. Hence, for the analysis of rarefied gas dynamics, the DSMC method has proved to be a very powerful tool.

Most applications of the DSMC have used \textit{structured grids} [5] to discretize the physical domain. For problems
with complicated geometry, multi-block meshing techniques were developed first by Bird [5], which involved two
steps: dividing the flow field into several blocks followed by discretizing each block into quadrilateral (2-D) or cubic
(3-D) meshes. Subsequent research has been directed to develop alternative meshing techniques such as the
coordinate transformation method by Merkle [15]. However, all of these still used structured grids. It is much easier
to program the code using structured grids, however, it requires tremendous problem specific modification. To
alleviate such restriction, an \textit{unstructured grid} system is an alternative choice, although it might be computationally
more expensive. Boyd's group [9] has applied such techniques to compute thruster plumes produced by spacecraft
and found that the results are very satisfactory. Wilmoth et al. [11] have used two types of grid (unstructured
tetrahedral and structured Cartesian grids) to compute the low-density, hypersonic flows about reusable launch
vehicle. Both methods were shown to give comparable results; however, it was concluded that unstructured grid
offers certain advantages for grid refinement and structured grid appears to offer greater overall advantages.

Wong and Harvey [16] have further employed re-meshing adaptive grid techniques in combination with
unstructured meshes to study flows with highly non-uniform density. However, the above-mentioned studies were
mostly applied to high-speed gas flows.

For low-speed gas flow applications, Pickos and Breuer [12] used DSMC to analyze the gas dynamics of micro-
mechanical devices using unstructured grids. In their research, they developed a special way to accommodate the
inflow/outflow pressure boundary conditions. Nance et al. [13] adopted the theory of characteristics from continuum
gas dynamics and incorporated the procedure in the DSMC method to handle the pressure specified micro-channel
gas flows at a subsonic exit. However, the treatment of the exit pressure boundary was based on the assumption that
the gas flow at the exit is adiabatic and isentropic, which is doubtful for most internal gas flows.

Alexander et al. [17] used DSMC to simulate the nano-scale gas flow of a computer hard drive slider air bearing.
The results showed that the gas pressure inside the air bearing is not uniform. In treating these pressure boundary
conditions, they have also designed a special way to update the inlet and exit speeds such that the inlet and exit
pressures are the same as specified. However, it is not clear how they precisely implemented the treatment.

Recently, Wu et al. [14] developed an effective way to process pressure boundaries with the DSMC method and
successfully applied it to gas flows with simple geometries such as micro-channel and backward-facing micro-step
configuration. The developed pressure boundary treatment is inherently mass conserved because particle flux
conservation is applied at each pressure boundary, assuming thermal equilibrium. Also it has been demonstrated [14]
that the procedure requires fewer time steps to “converge” to the steady-state solution as compared with the
approach of Nance et al. [13]. However, their application to gas flows with more complicated geometry or with
many inlets and exits are yet to be verified. In addition, it is also crucial to understand its limit of applicability in
rarefied or micro-scale gas flows.

From the previous review, we see a need to develop an efficient and accurate simulation/analysis tool for
thermal/fluid problems in micro-scale gas flows with pressure boundaries. Thus, the objectives of the current
research are to develop a DSMC code using an unstructured grid system and to apply the code to several micro-scale
gas flows, including micro-manifold, micro-nozzle and computer hard drive slider air bearing by using the pressure
boundary treatment developed previously [14].

\section*{NUMERICAL METHOD}

Due to the expected rarefaction caused by the very small size of micro-scale or nano-scale devices, the current
research is performed using the DSMC [5] method, which is a particle-based method. The basic idea of DSMC is to
calculate practical gas flows through the use of a method that has a physical rather than a mathematical foundation.
The assumptions of molecular chaos and a dilute gas are required by both the Boltzmann formulation and the DSMC
method [5]. The molecules move in the simulated physical domain so that the physical time is a parameter in the
simulation and all flows are computed as unsteady flows. An important feature of DSMC is that the molecular
motion and the intermolecular collisions are uncoupled over the time intervals that are much smaller than the mean
collision time. Both the collision between molecules and the interaction between molecules and solid boundaries are
computed on a probabilistic basis and, hence, this method makes extensive use of random numbers. In most
practical applications, the number of simulated molecules is extremely small compared with the number of real molecules. The details of the procedures, the consequences of the computational approximations can be found in Bird [5]. In the current study, the Variable Hard Sphere (VHS) molecular model [5] and the No Time Counter (NTC) [5] collision sampling technique are used to simulate the molecular collision kinetics except for the case of computer hard disk slider air bearing problem. Note that the corresponding molecular data including reference diameter ($d_{ref}$), reference temperature ($T_{ref}$), and the viscosity temperature exponent ($\gamma$) for each species are taken from those listed in Ref. 5. Solid walls of all cases considered in this study are assumed to be fully diffusive (100% thermal accommodation) and are equal to 300K unless otherwise specified.

In order to perform accurate simulation for inflow/outflow pressure boundaries, general procedure for treating these conditions by using the concept of particle flux conservation has been developed and incorporated into the basic DSMC algorithm [14]. The basic idea is to update the inflow and outflow velocities by applying particle flux conservation, assuming thermal equilibrium, at each pressure boundary, such that the mass flow rate conserves automatically and the simulated boundary pressures coincide with the imposed values. By applying the above procedures at the inflow and outflow pressure boundaries, the simulated inflow and outflow pressures are found to be consistent with the specified inflow and outflow pressures and mass conservation holds as well automatically. In Ref. 14, the results of a micro-channel flows using the current approach agreed very well with those of Nance et al. [13] and it was shown that fewer samplings are required to “converge” to the steady-state solution.

The macroscopic quantities such as mean velocities and temperature are sampled and averaged from cells, which may be triangular, quadrilateral or hybrid with both. Because of the unstructured meshes used, cell-by-cell particle tracing technique similar to Piekos and Breuer [12] is adopted to locate the final particle position at the end of each time step during computation. This might increase the computational load in locating the cell number of the final particle position during each time step, however, it offers the greatest flexibility of handling different types of boundary conditions and required much less problem specific change in programming. In practice, the computational time required using a particle tracing technique is comparable to those of structured mesh with careful selection of time-step and cell sizes using the same number of simulated particles.

RESULTS AND DISCUSSION

T-shaped Micro-manifold

A micro-manifold is chosen as the first application case for the purpose of testing the general treatment of pressure boundaries with multiple exits, a device with potential applications in medical technology. The sketch of a T-shaped micro-manifold is shown in Fig. 1 with one inlet and two exits, where exit 1 is at the upper right hand side (horizontal channel) and exit 2 at the lower bottom side (vertical channel). For the current simulation, $L/h_i=7$, $H/h_i=3$, $h_i=h_{o1}=h_{o2}$ and $h_e=1\mu m$. The inlet pressure is fixed and the pressures at exit 1 and 2 are varied such that the pressure ratios between the inlet and exits are 3:1:1 (case I), 3:1:2 (case II) and 3:2:1 (case III), respectively. Argon is the working gas with the inlet value (uniform) of temperature and pressure equal to 300K and 26.79kPa, respectively. The resulting Knudsen number based on the inlet conditions is 0.2. The initial conditions inside the micro-manifold are set as follows: zero mean velocities, uniform temperatures as $T_i$ and uniform number densities as the inlet value. The time step used is $8.33E-11s$.

Typical normalized mass flow rates as a function of time are presented in Fig. 2 for the case of specified pressures, $P_i:P_{o1}:P_{o2}=3:1:1$ (case I). This illustration monitors how the mass flow rate at each pressure boundary converges to its steady value and how the total mass flow conserves as well. Before the sampling starts, the mass flow rates at the inlet and exits fluctuates violently (sometimes negative, not shown in the figure); however, after the sampling starts, the corresponding mass low rates begins to converge to the steady values. Sum of the exit flow rates is greater than the inlet flow rate before reaching steady state (for time less than approximately 0.01 seconds in Fig. 2) is because of the initial conditions imposed. The larger mass flow rate of the sum of the exits initially is caused by the larger difference between initial flow field density (the same as inlet value) and the initial value of the exit density value. We have tried different initial conditions by varying the initial uniform density in the flow field from vacuum (lowest) to inlet value (highest). As expected, the final steady state mass flow rates are the same for all cases. By applying the particle flux conservation at each pressure boundary, the mass flow rate summation of exits 1 and 2 quickly approaches the mass flow rate of the inlet, within 0.6% in this case. Also about 54% of the mass flows out of exit 1 (horizontal channel). This behavior is mainly due to the larger pressure drop required for the gas particles to turn into the vertical exit 2. Consequently, the mass flow rate is less at exit 2, as illustrated in Fig. 2.

General flow properties for the T-shaped micro-manifold, including u-velocity and v-velocity contours, are
illustrated in Fig. 3 with $P_i: P_{el}: P_e=3:1:1$. From Fig. 3, we can see that gas flow accelerates gradually in the horizontal channel and achieves maximum speed at about 0.17 times the most probable speed based on inlet conditions, $c_{mp}$, at the turning corner and then decelerates rapidly across the corner region and finally accelerates gradually again further downstream in the horizontal channel with a centerline exit speed at about 0.17$c_{mp}$. Similarly, the gas flow from the inlet of the horizontal channel accelerates across the corner region down to the exit 2 in the vertical channel with a smaller centerline exit speed (about 0.15$c_{mp}$) than that of exit 1. However, at this flow condition with the same pressures at both the exits, more gas particles flow into exit 1 than exit 2 (about 8% more, as discussed earlier) since a higher pressure drop for the gas flowing into exit 2 is required at the turning corner (larger pressure gradient). Also appreciable slip velocities at the solid wall, in the range of 0.06-0.12 $c_{mp}$, are observed at the inlet Knudsen number of 0.2. Although there is no direct experimental data or theoretical prediction available to support the simulation conducted in the T-shaped micro-manifold, the physical trends qualitatively coincide with physical expectation. Thus, the generality of the pressure boundary treatment, using particle flux conservation, for multiple inlet and exits is at least qualitatively established.

**Micro-nozzle**

A micro-nozzle is selected as the second tested case because of its complex geometry and its potential for application as a MEMS device-- micro-thrusters on spacecraft, for example. Additionally, this might serve as a test case to identify the limit of applicability of pressure boundary treatment [14], assuming thermal equilibrium, and results are presented later that clearly identify the problems at large Knudsen number flows. A micro-nozzle with area ratio (ratio of inlet to throat area; AR, hereafter) of 2 is considered. The dimensions are shown in Fig. 5. L/h=6.0, where L and h are the nozzle length and throat height, respectively, and $h=1\mu m$. The inlet pressure, $P_i$, remains fixed at 80.4kPa, while the specified exit pressure, $P_e$, is reduced such that the resulting pressure ratio of exit to inlet ranges from 0.667 to 0. The “ 0 ” case refers to vacuum specified at the nozzle exit. Again, argon is used as the working gas. The resulting Knudsen number based on the inlet conditions is 0.067, while that based on exit conditions (simulated) is in the range of 0.098-0.537. For the vacuum case, any particles crossing the exit boundary during simulation are removed and no particles are introduced from outside this boundary, while at inlet pressure boundary particle flux conservation is imposed. Figure. 5 illustrates the Mach number contours in micro-nozzle in the order of decreasing exit pressure with the same inlet pressure. It is clearly that the exit Mach number increases with decreasing pressure ratio as expected. From Fig. 5, the centerline Mach number increases along the nozzle, a maximum value is obtained at the downstream side of the nozzle throat and then decreases further downstream in the diverging section of the nozzle. Note that the position of maximum Mach number moves further downstream as the exit pressure decreases. The exit Mach number is still subsonic for $P_e/P_i \geq 0.2$. This is obviously different from the continuum analysis, assuming a quasi-1-D inviscid flow, due to the viscous effects and strong rarefaction [10]. In Fig. 6b, with $P_e/P_i=0.20$, the centerline Mach number increases all the way from the converging section to the diverging section, and a substantial Mach number, $M_e=0.74$, is observed at the exit center. In the case of a vacuum exit (Fig. 6c), supersonic speed with Mach number of approximately 1.25 is obtained; however, as expected, it is much lower than the Mach number of 1.73 predicted from continuum analysis. The data presented in Fig. 6a fluctuate more than the other due to the lower speed involved and the inherent statistics used in the DSMC method. The situation improves as pressure ratio decreases (hence, the speed increases). Appreciable slip velocities are observed along the nozzle walls. For the vacuum exit condition, Mach numbers of the order of 0.70 close to the exit are observed (Fig. 6c). The most striking features with micro-nozzle flows is that there is no shock predicted inside the diverging part of the nozzle, as would be expected from 1-D inviscid continuum analysis, for all the exit pressures considered. The absence of shocks might be due to the strong viscous and rarefaction effects, which deserves further study.

Temperature contours in the order of decreasing pressure ratio are shown in Figs. 6a-6c. Fig. 6a exhibits a high degree of scatter for the lower pressure ratio case, the reason are due to the low speed flows involved and the large statistical variance of the instantaneous particle velocities used in obtaining the temperature data. Temperature distribution obviously is not uniform in both spatial directions, especially in the diverging part of the nozzle. Temperature tends to decrease along the nozzle due to flow acceleration (gas expansion) as shown clearly in Figs. 6b and 6c. In addition, the exit temperature decreases with decreasing pressure ratio and can be as low as 0.66 times the inlet temperature, as is the case for the vacuum exit condition. Temperature jump in the converging part of the nozzle is negligible; while it becomes substantial in the diverging part of the nozzle due to the high local Knudsen number close to the walls. For example, temperature jump can grow to 0.11 times that of the inlet temperature with a vacuum exit, as shown in Fig. 6c.
Fig. 1 Sketch of T-shape micromanifold 
(h₁=he₁=he₂, L/H=7/3, L/h₁=7, Kn₁=0.2).

Fig. 2 The contour plots of micro-manifold with 
P₁:Pₑ₁:Pₑ₂ = 3:1:1 (a) u-velocity (b) v-velocity

Fig. 3 The normalized mass flow rate for a T-shape micromanifold with 
P₁:Pₑ₁:Pₑ₂ = 3:1:1

Fig. 4 Sketch of micro-nozzle (AR=2, L/h=6).

Fig. 5 Mach number contours of micro-nozzle at different pressure ratios with 
Pₑ/P₁ equal to (a) 0.667 (b) 0.20 (c) 0 (Knₑ=0.067, AR=2).

Fig. 6 Temperature contours of micro-nozzle at different pressure ratios with 
Pₑ/P₁ equal to (a) 0.667 (b) 0.20 (c) 0 (Knₑ=0.067, AR=2).
The main purpose of choosing a slider air bearing as the final tested case is because of the availability of similar simulation data available in the literature and the opportunity to test pressure boundary treatment for a moving wall. In addition, this inherently high Kn number test case, also serves to identify the applicability limits of the pressure boundary treatment. The test configuration, as shown in Fig. 8, is the same as that in Alexander et al. [17] and is briefly described as follows. A hard sphere Argon gas (d_{re}^0.366nm; α=0.5) with T_i=273K; fixed height ratio, h_{hi}/h_e=2 (L/h_e=100), and Ma=0.08 (Kn_{ni}=0.625; h_e=50nm), 0.50 (Kn_{ni}=2.084; h_e=15nm) and 1.0 (Kn_{ni}=0.625; h_e=50nm). Note that T_i is the inlet gas temperature, h_i is the inlet height of air bearing, h_e is the exit height of air bearing, L is the length of the platter, Ma is the Mach number defined by the platter speed and inlet acoustic speed, and Kn_{ni}=λ/h_e. Although the inlet and exit pressures are both at atmospheric level (P_0), it is highly rarefied due to the nano-scale gap between the write/read head and the rotating disk.

Present simulated centerline gas pressure profiles are presented in Fig. 8 along with those obtained by Ref. 17 for comparison, where x/L is the nondimensional location in the platter moving direction. Note that the data illustrated as lines are present simulated centerline gas pressures, while the solid symbols are present simulated wall pressures, obtained by the summation of incident and reflective momentum of particles on the write/read head surface, and the open symbols are gas pressures obtained in Ref. 17. Note that gas pressure is obtained using ideal gas law, where total average temperature is used. As can be seen, the present simulated gas pressure profiles are in good agreement with those in Ref. 17 for all three cases considered. Note that only gas pressures are reported in Ref. 17. All the predicted pressures increase at first along the air bearing, achieving the maximum values, and then decreasing rapidly at the end of the air bearing. The initial rate of increase of the gas pressures is essentially the same for Ma>0.5, while the rate of decrease after the maximum pressure and the maximum value both increase with Mach number.

For a low rotating disk speed, Ma=0.08, the present predicted wall pressures agree well with predicted gas pressures. This means that at low rotating disk speed, the gas particles are in thermal equilibrium, and hence the gas pressures are isotropic, resulting in the same pressure distribution both at wall and in the gas. However, at Ma=0.5 and Kn_{ni}=2.08, obvious discrepancies are observed between the present predicted gas pressures and the wall pressures. The present predicted wall pressures are generally lower than the present predicted gas pressures especially those at the inlet region. This discrepancy increases as Ma increases. The deviations between the gas pressures and the wall pressures are due to the fast moving platter speed and the highly rarefaction of the flow. Particles entering from the inlet are entrained to collide with the moving plate at the bottom such that substantial downward mean velocities (v-velocities) are formed at the inlet region. Therefore, there are comparatively fewer particles from outside the inlet colliding with the upper wall, especially near the inlet. This trend of deviation is more clear for the higher Mach number case, Ma=1.0. This difference can be explained partly next by the non-equilibrium between different translational temperatures in the gas.

Figure. 9 presents the predicted ratios of translational temperature, T_x/T_y, as a function of non-dimensional location, x/L, at Ma=0.08, 0.5 and 1.0. For low disk rotating speed, T_x/T_y is nearly unity, which means the flow is in thermal equilibrium. As the disk rotating speed increases up to Ma=0.5, T_x/T_y attains a value of approximately 1.06, which represents a slightly non-equilibrium gas flow. A stronger non-equilibrium gas flow occurs as Ma=1.0 with T_x/T_y equal to 1.15. These non-equilibrium gas flows at high rotating disk speeds explains why the wall pressures are less than the gas pressures inside the air bearing since the gas pressures are obtained by averaging the translational temperatures (hence pressures) in three directions.

CONCLUSIONS

This investigation has successfully developed a DSMC code using unstructured meshes. The code is verified by comparison with theoretical equilibrium collision frequency and with previous results for the temperature profiles of a 1-D normal shock. The code is then used to test the general pressure boundary treatment developed previously [14] by applying it to three different typical micro-scale (or nano-scale) gas flows, including a T-shaped micro-manifold, a micro-nozzle and a slider air bearing of computer hard drive. The major conclusions of the study are as follows.

1. The developed code is highly flexible in handling flow fields with complicated geometry without much program modification.
2. The pressure boundary treatment of Ref. 14, assuming thermal equilibrium and applying particle flux
1.1 Motionless read/write head

Fig. 7 Sketch of slider air bearing (L/h_c=100, h_i/h_e=2, P_i=P_e=1atm).

2.2

Fig. 8 Gas pressure profiles for slider air bearing at different Knudsen numbers and Mach numbers.

2.0

Fig. 9 Ratio of temperature components, T_x/T_y, as a function of x-position in slider air bearing for different Mach numbers (L=5 μm for case I and case III, and L=1.5 μm for case II).

0.0

Fig. 9 Ratio of temperature components, T_x/T_y, as a function of x-position in slider air bearing for different Mach numbers (L=5 μm for case I and case III, and L=1.5 μm for case II).
conservation, is proved successful in computing gas flows with complicated geometry, multi-exits and moving boundary at low local Knudsen numbers. However, a clear criterion for the applicability of the equilibrium Maxwell-Boltzmann distribution function requires further study.

3. Simulated results of a T-shaped micro-manifold, a micro-nozzle and a nano-scale slider air bearing show that the application of particle flux conservation at pressure boundaries are successful for subsonic flows.

4. For a micro-nozzle flow, the over-prediction of exit pressure becomes appreciable as the $Kn_{ua}$ and $Kn_{Tu}$ exceed approximately 0.05; however, the deviation is negligible at similar values of $Kn_{ua}$ and $Kn_{Tu}$ for slider air bearing. This suggests that the applicability of the current pressure boundary treatment depend not only on $Kn_{ua}$ and $Kn_{Tu}$ but also on the interface speed at the pressure boundary.

This study raises the question of using the equilibrium Maxwell-Boltzmann distribution function in highly non-equilibrium gas flows. Thus, more studies towards resolving the above concern is worthwhile and are currently in progress.

REFERENCES