Study Of Low Speed Transitional Regime Gas Flows In Microchannels Using Information Preservation (Ip) Method

Umit Kursun
University of Central Florida

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STUDY OF LOW SPEED TRANSITIONAL REGIME
GAS FLOWS IN MICROCHANNELS USING
INFORMATION PRESERVATION (IP) METHOD

by

UMIT KURSUN
Bachelor of Science, Bogazici University, 1999
Master of Science, Bogazici University, 2001

A dissertation submitted in partial fulfillment of the requirements
for the degree of Doctor of Philosophy
in the Department of Mechanical, Materials and Aerospace Engineering
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Major Professor: Jayanta S. Kapat
ABSTRACT

Proper design of thermal management solutions for future nano-scale electronics or photonics will require knowledge of flow and transport through micron-scale ducts. As in the macro-scale conventional counterparts, such micron-scale flow systems would require robust simulation tools for early-stage design iterations. It can be envisioned that an ideal Nanoscale thermal management (NSTM) solution will involve two-phase flow, liquid flow and gas flow. This study focuses on numerical simulation gas flow in microchannels as a fundamental thermal management technique in any future NSTM solution. A well-known particle-based method, Direct Simulation Monte Carlo (DSMC) is selected as the simulation tool. Unlike continuum based equations which would fail at large Kn numbers, the DSMC method is valid in all Knudsen regimes. Due to its conceptual simplicity and flexibility, DSMC has a lot of potential and has already given satisfactory answers to a broad range of macroscopic problems. It has also a lot of potential in handling complex MEMS flow problems with ease. However, the high-level statistical noise in DSMC must be eliminated and pressure boundary conditions must be effectively implemented in order to utilize the DSMC under subsonic flow conditions.

The statistical noise of classical DSMC can be eliminated through the use of IP method. The method saves computational time by several orders of magnitude compared to a similar DSMC simulation. As in the regular DSMC procedures, the molecular velocity is used to determine the molecular positions and compute collisions. Separating the
macroscopic velocity from the molecular velocity through the use of the IP method, however, eliminates the high-level of statistical noise as typical in DSMC calculations of low-speed flows.

The conventional boundary conditions of the classical DSMC method, such as constant velocity free-stream and vacuum conditions are incorrect in subsonic flow conditions. There should be a substantial amount of backpressure allowing new molecules to enter from the outlet as well as inlet boundaries. Additionally, the application of pressure boundaries will facilitate comparison of numerical and experimental results more readily.

Therefore, the main aim of this study is to build the unidirectional, non-isothermal IP algorithm method with periodic boundary conditions on the two dimensional classical DSMC algorithm. The IP algorithm is further modified to implement pressure boundary conditions using the method of characteristics. The applicability of the final algorithm in solving a real flow situation is verified on parallel plate Poiseuille and backward facing step flows in microchannels which are established benchmark problems in computational fluid dynamics studies. The backward facing step geometry is also of practical importance in a variety of engineering applications including Integrated Circuit (IC) design. Such an investigation in microchannels with sufficient accuracy may provide insight into the more complex flow and transport processes in any future Nanoscale thermal management (NSTM) solution. The flow and heat transfer mechanisms at different Knudsen numbers are investigated.
Dedicated to my dear parents

NADIDE and ZEKI
ACKNOWLEDGMENTS

All praises belong to Allah, the Creator and Sustainer of the universe.

I am thankful to my Lord for allowing me to earn my Doctoral Degree in Mechanical Engineering from a department with outstanding faculty members in a top-rated university, University of Central Florida. Obtaining this degree in the States has been definitely the utmost learning experience for me, which I will always remember and utilize in my career in the future.

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I would like to thank to my dear professors and members of my dissertation committee, Departmental Chair Dr. Ranganathan Kumar, and Dr. Fang Xu, Dr. Quanfang Chen, and Dr. S. Roy Choudhury from the Mathematics Department for their time, interest, valuable input and suggestions.
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LIST OF VARIABLES

a  speed of sound

C_κ, C_μ  numerically determined coefficients

F_c  number flux through a boundary or a cell

k  Boltzmann coefficient

Kn  Knudsen number

n  number density

N  sampling size

N_t  number of molecules inside the cell at a given time step

N_{TS}  number of time intervals between two samples

p  pressure

q''  heat flux per unit channel width

R  gas constant

T  temperature

T_1, T_2  pre-collision temperatures

u, v, w  velocity components

V  molecular speed

V  molecular velocity

V_0  mean flow velocity

V_1, V_2  pre-collision velocities

V_1', V_2'  post-collision velocities
$V_{mp}$  most probable thermal speed

$V_{th}$  random thermal velocity

$\rho$  density

$\zeta$  number of degrees of freedom
CHAPTER ONE: INTRODUCTION

Over the past two decades, the microsystems have evolved significantly. In parallel to the improvements in micro-device and system performance, the industrial demand for efficient, reliable, compact and light-weight systems has also increased dramatically. This however, has come at a price—the urgent need for better cooling techniques and a management framework that considers the entire system. It is now widely established that thermal management is an indispensable part of a design cycle. Proper design of thermal management solutions for future nano-scale electronics or photonics will require knowledge of flow and transport through micron-scale ducts. Continued improvements, otherwise, would most likely be challenged. In view of that, there is an urgent demand for a better understanding of the fundamentals of fluid mechanics and heat transfer on the microscale.

Navier-Stokes equations ignore the molecular nature of the fluids (gas and liquid) and regard them as continuous medium describable in terms of the spatial and temporal variations of density, velocity, pressure, temperature and other macroscopic bulk flow quantities. Continuum approaches with no-slip boundary condition at the solid fluid interface fail to give correct predictions for modeling the flows having the characteristics length scales as large as flow dimensions.
Modifications in the boundary conditions, transport coefficients or equation of state can help removing small discrepancies up to some extent. However, even for a simple case of acceleration-driven Poiseuille flow with relatively small gradients and Knudsen number, a correction throughout the whole system is not possible with these types of modifications (Zheng et al, 2002).

Numerous studies on fluid flow in microscale have well established that microscale fluid behavior is different from the conventional macroscale flows. On the other hand, none of these studies has clearly stated the exact reasons behind this phenomenon. The attempts to understand and model the physics and mechanism of micro flows have led serious discussions over the last decades that are still on going.

To determine the degree of rarefaction of a gas, the dimensionless Knudsen number Kn is used. The Knudsen number can be expressed as

\[ Kn = \frac{\lambda}{L} \]  

(1)

where \( \lambda \) is the mean free path and \( L \) is the characteristic length.

In order to specify a specific Kn for the complete flow, the dimension, \( L \), can be defined as the overall length of the flow. However, a local Kn is often used as it is more
appropriate for large or complex systems. In this case, $L$ is defined as the length scale of a macroscopic gradient such as density, temperature, pressure, or velocity within the flow.

The mean free path for a gas molecule is the average distance traveled by a molecule before colliding to another molecule. Since the mean free path is directly proportional to temperature but inversely proportional to pressure, it can go up to several meters in the upper atmospheric levels.

In kinetic theory of gases the mean free path is defined as the ratio of mean thermal speed to collision frequency.

Using the hard sphere molecular model, the mean free path can be expressed as

$$
\lambda = \frac{1}{\sqrt{2n\sigma}}
$$

(2)

where $\sigma$ is the effective collision cross section and $n$ is the number density. At the standard atmospheric pressure and at a temperature of 20 °C, air molecules have a mean free path of 68 nm. The following table summarizes the categorization of flow regimes based on Knudsen number.
<table>
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<th>Flow Regime</th>
<th>Kn</th>
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Atmospheric gas dynamics (space craft reentry) and materials processing (plasma-etch applications) are important fields which deal with quite low gas densities while the relatively new, the MEMS technology, deals with relatively high gas densities in microchannels. Being more than a scientific interest, the practical applications in all these fields require the full understanding of high-\text{Kn} flows.
The Navier Stokes equations are derived under the assumptions of local equilibrium for flows with small gradients and low Kn numbers. The validity of Navier Stokes can be extended by using slip and jump boundary conditions. However, the convergence depending on Reynolds number may become a problem for microflows. And the slip flow assumption of one-dimensional Knudsen layer may not be valid for complicated flow geometries such as those involving corners, sharp edges, etc. More importantly, the Navier Stokes equations do not constitute a determinate set; thus breakdown of the continuum occurs when the local Kn becomes greater than 0.1 depending on the flow properties. Beyond this approximately defined regime, the intermolecular collisions have
the same order of probability as the molecule-wall collisions. In this regime, high
gradients near walls and other surfaces are believed to affect the flow in ways different
than those visible in larger systems. Therefore, a molecular model must be employed
instead of the traditional continuum models and numerical techniques.

The deterministic approaches such as the Molecular Dynamics (MD) methods are the
best known particle based algorithms. In MD simulations, the time step in the simulation
is limited by the time scales of the interaction potential and the solution method. If the
working fluid is chosen as a dilute gas, it could take millions of time steps to calculate a
few molecular collisions.

The total computational time needed by MD is proportional to the square of the simulated
particles since trajectories of all particles in the system must be followed to determine
collisions and the potential function.

Therefore, despite the developments in the computational resources, MD simulations are
still impractical for simulations lasting more than a few nanoseconds of time and a few
nanometers in the spatial domain.

The realistic and practical problems that incorporate the complex geometries,
representing the interaction of multi species and considering the radiation effects are
beyond the capabilities of the current technology to solve with MD.
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Time dependent, nonlinear Boltzmann equation is a fundamental equation of gas kinetic theory. It is valid for all flow regimes if the collisions occurring in the gas are binary or two-body collisions.

The Boltzmann equation can be expressed as:

\[
\frac{\partial n f}{\partial t} + \mathbf{v} \cdot \frac{\partial n f}{\partial \mathbf{r}} + \mathbf{F} \cdot \frac{\partial n f}{\partial \mathbf{V}} = \int_{-\infty}^{+\infty} n r (f^+ f^- - f f^*) \mathbf{V}, \sigma d\Omega d\mathbf{V} \tag{3}
\]
where \( f \) is single-particle velocity distribution function, \( n \) is the number density, \( \mathbf{V} \) is the molecular velocity, \( V_r \) is the relative speed, \( \mathbf{r} \) is the space vector, \( \mathbf{F} \) is the external force vector per unit mass, \( \sigma \) is effective molecular collision cross section, \( \Omega \) is the solid angle and prime symbol refers to post-collision values of the colliding class of molecules.

Basically, the Boltzmann equation evaluates the rate of change in the number of molecules in space due to contributions of advection, external force field and molecular collisions. A macroscopic quantity can be evaluated by proper integration of the corresponding microscopic quantity provided that the velocity distribution of particles is known.

Using small perturbation theory, the Boltzmann equation can be solved in closed form by assuming the distribution function in power series expansion as

\[
f = f(0) + Kn f + Kn^2 f^2 + \ldots
\]  

(4)

The first term of the expansion is the Maxwell or local equilibrium distribution function which can model an isentropic flow. Therefore, when \( Kn \) is zero in the limit, the expansion equation reduces into the inviscid Euler equations.
For a Knudsen number much less than the unity, the flow attains a continuum where gas phase collisions are important. Although the velocity distribution departs from the ideal Maxwellian, the changes in the transport coefficients are still negligible. The second term in the expansion leads to Navier Stokes, showing that the Navier-Stokes is valid to the first order Kn.

For Kn less than 0.1, velocity slip and temperature jump at the wall must be taken into account by using modified boundary or solid wall slip conditions. Arkilic et al (2000) have shown that, for a long, high-aspect ratio microchannel with isothermal diffusive walls, the velocity slip at the wall can be given by

$$u_w = \alpha \lambda \frac{du}{dy}|_w$$

where $u$ is the streamwise velocity, $\lambda$ is the mean free path, and $\alpha$ is a surface-dependent coefficient. In the study, the streamwise pressure distribution is also formulized in terms of Knudsen number at the channel-outlet and the pressure ratio.

Beskok and Karniadakis (1994) employed high order equations to advance this methodology. However, the Navier-Stokes equations are strictly valid only to first order in Kn as can be seen from the expansion equation above.
The third term in the expansion points to Burnett equations. The available methods are introduced by Burnett (1936) and Grad (1949). Burnett equations are obtained by simplifications of the high-order stress tensor and heat flux terms using isentropic relations. It is also possible to obtain the Burnett equations from Grad’s 13-moment equations under certain conditions.

As mentioned earlier, for Knudsen numbers larger than 0.1, the flow modeling cannot be done with continuum methods successfully. After the Knudsen number reaches the unity, there is no alternative approach to particle methods (Bird, 1978).

The only equation can be used in closed form is then the Boltzmann Equation with assumptions. Analytical solutions for infinitely large Knudsen numbers are available in the free-molecular flow regime. However, at finite Knudsen numbers, serious difficulties emerge in the analytical solution limiting the problems that can be solved. Direct numerical solution of Boltzmann equations is also very difficult since the computer power required to model velocity distribution in the three dimensional physical space and the collision integral is beyond the capabilities of the current computer resources.

When Boltzmann solution is not practical, for instance in studying the characteristics of strong shock waves (Liepmann, 1962), the simplified models are used. The simplification of the Boltzmann equation may be done by linearization of the collision integral for flows in which average speed and temperature slightly vary (Cercignani 1975). Alternatively,
the source term in the Boltzmann equation can be simplified as in BGK approximation (Bhatnagar et al 1954). In this model, the molecular collision frequency depends on temperature instead of molecular velocity. Also a direct solution is obtained by Hicks-Yen-Nordsieck through a hybrid approach employing both Monte Carlo and finite difference techniques (Nordsieck & Hicks 1967, Yen 1971) to solve Boltzmann equation.

There are other studies in the literature. However, these methods do not yield accurate results for highly nonlinear problems. The problems involving large disturbances, complex molecular models and several independent variables cannot be handled practically with Boltzmann Equation.

Unlike the Navier-Stokes equations which assume the fluid is a continuum, the probabilistic methods take the discrete particles or molecules into account to simulate the fluid. Being different than MD methods, these probabilistic Monte Carlo methods do not track particles or compute molecular collisions in a deterministic manner. However, the statistically generated solutions are consistent with the Boltzmann formulation. Rather than physical reasoning, the derivation of DSMC algorithms from the Boltzmann equation is proved by Nanbu (1988) for a monoatomic gas experiencing binary collisions.
**Direct Simulation Monte Carlo Method**

The Direct Simulation Monte Carlo, DSMC, proposed by G.A. Bird (1994) is a statistical particle method based on kinetic theory. Due to its conceptual simplicity, the DSMC method has been developed and widely used as a powerful and primary tool to study and simulate the dynamics of gas flow at any gas rarefaction for which the continuum assumption is not valid.

As stated earlier, especially for the hypersonic flows where high non-equilibrium effects are present, the DSMC is the primary solution method of choice.

In contrast to general computational fluid dynamics studies, the DSMC do not solve Boltzmann equations mathematically. However, being consistent with Boltzmann formulation, the collisions are generated stochastically and post-collision states are determined using kinetic theory of dilute gases. Therefore, the method can handle complicated practical flow solutions with ease.

The DSMC is valid for all Kn regimes. It, however, becomes computationally expensive to use DSMC for very low values of Kn. The most suitable regime for DSMC simulations is the transition regime where the Kn is between the order of 0.1 and the order of 10.
As can be seen from Eqn. (1), a large Kn may result either from a large mean free path or from a small length scale of the macroscopic gradients. The former condition, a large mean free path is usually a consequence of a very low gas density whereas the latter can be encountered in the internal structure of a shock wave which requires a molecular model at all densities.

Figure 2. Regimes of validity of the solution methods

For a fixed molecular diameter, d, as the molecular spacing, \( \delta \), decreases the density increases. Hence, a fluid is said to be dilute when the ratio of the molecular spacing, \( \delta / d \) is much larger than the molecular diameter, d.
For a dilute fluid, when the ratio of mean free path to the molecular diameter, $\lambda/d$, is larger than 10, the Direct Simulation Monte Carlo method may be used efficiently. However, the number of simulated particles per volume, thereby, the number of molecular collisions should be high enough.

As in classical kinetic theory, the molecular chaos is assumed and only binary collisions are considered. Therefore, the theory restricts the use of DSMC to dilute gases where the molecular spacing is large compared to the molecular diameter. Although, this statement is given by the inventor of the code, Bird (1988), more recent studies (Morris et al 1992, Cheng 1993) have shown that the DSMC method is capable of producing solutions close enough to that of Navier-Stokes for very low Knudsen numbers.

Unlike CFD techniques, the DSMC does not have any stability criteria. Nevertheless, in order to obtain accurate results out of classical DSMC method, there are some theoretical requirements. Otherwise, resulting mean flow properties may suffer from high statistical fluctuations.

**Principles of DSMC**

The DSMC is a simulation method based on kinetic theory which is equivalent to solving the Boltzmann equation for a monoatomic gas having binary collisions.
The main idea of DSMC is reducing the real number of the molecules by using a reduced number of simulation particles and uncoupling their movement and collisions. Generally the number of simulation particles is around $10^4$-$10^5$ each representing a large number of real particles. The deterministic molecular motion and stochastic intermolecular collisions are uncoupled by use of a small time interval $\Delta t$. The time step must be smaller than the real physical collision time estimated by the kinetic theory for getting accurate results. This is a physical requirement rather than a numerical stability criterion. Additionally, if the time step is small enough, a particle also spends enough time in a cell to interact with other particles before exiting that cell. The numerical results do not depend on the amount of the time step as long as this criterion is satisfied.

The spatial domain is divided into the net of cells which are used for selection of collision partners and obtaining macroscopic flow quantities. A rectangular cell structure is employed in this study although unstructured, body-fitted cell geometries can be incorporated as long as tracking of particles is possible.

The linear dimension of cell $L_c$ can not be longer than the mean free path. Usually the length of the cell is chosen about one third or one fourth of the mean free path. Setting cell sizes larger than the mean free path cause an under-prediction of the macroscopic gradients. When the sub-cells are used in the cells to help reduce the distance between the collision partners, the cell size restriction applies to them rather than cells.
The simulation particles are indexed and sorted into these cells. Initially assigning 20-40 simulation particles per cell is a common practice. Decomposition of the flow domain by cells facilitates evaluating the macroscopic flow properties and calculation of the molecular collision process.

![Computational grid consists of rectangular cells](image)

Figure 3. Computational grid consists of rectangular cells

Based on the definition of the problem, symmetry planes can be used in order to reduce the number of cells and data storage. Regardless of that, the kinetic theory of gases requires consideration and calculation of all the three components of the velocity in molecular collisions.

Since the side length of a cell must be less than mean free path at the given conditions, the time step $\Delta t$ must be selected such that there will be no particle traveling over a length of a cell in one time step. Although the results does not depend on the time step, an
appropriate time step must be provided for a given velocity input fulfilling this requirement.

**How DSMC Works**

The working principal of DSMC consists of four main steps: moving the simulated particles, indexing and sorting them, evaluating the collisions statistically, and sampling the flow field.

In the beginning, the simulated particles are randomly distributed in cells equally obeying the initial density requirements. Random thermal velocities of the particles are determined from a Maxwellian distribution. For each particle, an estimated mean flow velocity is added to the random thermal velocity for calculating total molecular speed. The inlet boundary condition is constant flow velocity for classical DSMC method. However, if one wants to specify pressures at the channel inlet and exit, specifying an inlet flow velocity as well as pressures would be over-specification of the problem. An example found in the literature is given in the section which explains application of pressure boundary conditions.

The first step of the simulation is the advection phase. Similar to MD simulations, the positions of the simulated particles are deterministically updated in a given time interval regardless of the possible interactions between.
The moving subroutine starts with calculating final positions of the particles by using the simple relation

\[ \tilde{x}_{f} = \tilde{x}_{i} + \tilde{v} * \Delta t \]  

(2)

where \( \tilde{v} \) is the particle velocity and \( x_{i} \) and \( x_{f} \) are initial and final positions respectively.

The number of new particles entering the flow from the domain boundaries is determined in this step by the kinetic theory of gases. Appropriate boundary conditions are enforced for these particles. In the classical DSMC algorithm, the particles exiting the flow domain are discarded. The external forces such as gravitation are taken into account and all necessary calculations required for the particles interacting with solid surfaces are also done here.

Since the solid-gas interaction is modeled by employing conservation laws for each and every simulation particles, physical, chemical and radiation effects can be incorporated into the algorithm easily.

The standard DSMC mainly employs three types of models to simulate gas-surface interaction: the simplistic specular reflection, more realistic diffuse reflection with thermal and momentum accommodation, and a combination of these two, the Cercignani-Lampis-Lord gas-surface interaction algorithm.
The specular reflection is a perfectly elastic collision of the particle with the solid wall. The normal component of velocity is reversed while the tangential velocity is kept the same. The time passes until the strike is subtracted from the total time interval, \( \Delta t \). After impingement, the particle continues its move with the new, updated velocity within the remaining time.

The specular model is not able to capture the boundary layers near the solid surfaces. Commonly used diffuse reflection gives more realistic results that are accurate enough for many engineering problems. In the diffuse reflection model, the solid wall temperature is used to evaluate all three components of the post collision velocities according to a half-range Maxwellian distribution regardless of the initial molecular velocity. This distribution is essentially biased since particles with higher speeds interact with the wall more often than the slow ones.

The final state of the particles after impingement can be correlated to that of pre-impingement depending on the value of the thermal and momentum accommodation coefficient. In the present study, the accommodation coefficient is equal to the unity. This is also known as the full thermal and momentum accommodation where there is no relationship exists between the pre- and post-impact states.

If the solid surfaces are not stationary as in Couette or Raleigh flows, the velocity of the wall is simply added to the reflection velocity of the particle.
Molecular indexing is the second step of the algorithm. Particles are tracked, grouped and sorted inside the cells and sub-cells. Using faster and more effective sorting algorithms would save computational time in this essential step.

The next step is simulating the collisions between the particles. The local collision rate of particles during a time step is calculated for each individual cell based on the kinetic theory of gases.

The collision pairs are randomly selected from those particles near each other inside the same cell or sub-cells if available. The sub-cell approach ensures that a collision occurs only if the colliding particles are close to each other.

The probability of a molecular collision does not depend on the position or trajectories of the candidate particles. Determining collision probability merely depends on the magnitude of relative velocity of candidate collision partners with respect to each other.

The collision of a candidate pair is accepted if their relative speed is large enough compared to the maximum relative speed in the same cell. This decision is made stochastically using an acceptance-rejection method.
A direct calculation which would increase the computational time enormously is avoided by intelligently guessing the maximum relative speed in the cell. To get an upper limit for the maximum velocity, the velocity distribution is sampled from time to time.

Figure 4. Classical DSMC Algorithm
The number of potential collisions per cell-volume per time then becomes

$$\Lambda = \frac{1}{2} N N F_N (\sigma C_r)_{\text{max}}$$  \hspace{1cm} (6)

where $N$ is the number of particles, the bar denotes time or ensemble averaging, $F_N$ is the number of real molecules represented by a single simulated particle, $\sigma$ is the effective molecular collision cross section, and $C_r$ is the relative speed of the particles colliding.

Post-collision quantities are computed in three dimensions regardless of the dimensionality of the computational domain. Four of the six equations needed come from linear momentum and energy conservation equations. Stochastic representations such as dilute gas hard or more realistic soft sphere potentials or rotational degrees of freedom are used to determine collision cross section as well as post collision velocities.

The hard sphere model can be considered as the idealistic collision of two spheres where the total momentum is conserved after the collision. The hard-sphere model does not represent real gas collisions accurately as the collision cross section is always constant.

The variable hard sphere VHS method is introduced by Bird (1988). Unlike the hard sphere model, the collision diameter is variable depending on the relative translational
energy during the collision. The method employs the viscosity-temperature power law based on a reference temperature and user-specified real-gas temperature exponent.

In the present study, variable cross-section hard sphere (VHS) method is employed. It is important here to note that the dynamic viscosity, mean free path, thus the Knudsen number, the time step, and other parameters used and presented in this study are all calculated and adjusted based on the VHS model.

After all of the steps are completed, the macroscopic physical quantities of interest can be sampled using ensemble averaging of the molecular information.

In this last step, the geometric centers of the cells are used for averaging the relevant information and interpreting these results in plots. The cell averaged density, mean velocity are calculated as follows

\[ \rho_c = \frac{\sum_{i=1}^{N} m_i}{Vol_c} \quad (7) \]

\[ \mathbf{v}_c = \frac{\sum_{i=1}^{N} m_i \mathbf{v}_i}{\sum_{i=1}^{N} m_i} . \quad (8) \]
In the kinetic theory of gases, the translational and rotational temperatures are defined for a gas in equilibrium as

\[ T_{tr} = \frac{2(mV^2 - mV_0^2)}{3k} \]  
\[ T_{rot} = \frac{2}{k} \left( \frac{\varepsilon_{rot}}{\zeta_r} \right) \]

where \( k \) is Boltzmann constant, \( m \) is mass of a gas molecule, \( V \) is molecular velocity, \( V_0 \) is the mean flow velocity. This definition is used without any change in DSMC even though the results produced by DSMC are for a system in non-equilibrium.

The translational and rotational energies of an individual molecule can be calculated as

\[ \varepsilon_{tr} = \frac{\sum_{i=1}^{N} \frac{1}{2} m |V_i|^2}{Vol_c} = \frac{3}{2} \frac{RT_{tr}}{m} \]

\[ \varepsilon_{rot} = -R_f(0)kT_{rot} \]

where \( \zeta_r \) is number of internal degrees of freedom, \( \varepsilon_{rot} \) is the rotational energy of a molecule and the over-bar denotes average, and \( R_f \) is a random number between 0 and 1, \( T_{tr} \) is translational temperature, \( T_{rot} \) is rotational temperature.
The Larsen-Borgnakke model with discrete rotational energy is used for modeling the energy exchange between translational and internal modes. For a diatomic gas, neglecting the vibrational energy, the temperature can be expressed as

$$T = \frac{3T_{tr} + \zeta \cdot T_{rot}}{3 + \zeta}$$  \hspace{1cm} (13)$$

where $T_{tr}$ and $T_{rot}$ are translational and rotational temperatures respectively.

The change in translational and rotational energy of the particles striking the wall gives the net heat flux on the wall that can be calculated as

$$q'' = F_N \frac{(\sum_{i=1}^{N_x} e_{i,pr} + \sum_{i=1}^{N_s} e_{i,rot})^{inc} - (\sum_{i=1}^{N_x} e_{i,pr} + \sum_{i=1}^{N_s} e_{i,rot})^{ref}}{\Delta x \cdot \Delta t}$$  \hspace{1cm} (14)$$

where $F_N$ is the real molecules represented by a single simulated particle, $N_s$ is the number of particles colliding to the wall, $\Delta x$ is the linear cell size, $\Delta t$ is the time passes between the beginning and the completion of the move in which the collision takes place, and the subscripts inc and ref represent incident and reflected states respectively.

If desired, the normal pressure and shear stress on the walls can be calculated from the time derivative of change in momentum. The pressure is defined as the net exchange of
the normal momentum fluxes of the incident and the reflected molecules at each time step per unit area of influence. Similarly, the tangential momentum on a horizontal plate can be calculated as

\[
\tau_w = \sum_{i=1}^{N_s} m(u_{i}^{\text{inc}} - u_{i}^{\text{ref}}) \over \Delta t \cdot \Delta A
\]  

where \( u \) is the velocity component of the particle parallel to the plate, \( \Delta t \) is the duration of the impact, \( \Delta A \) is the wall area, \( m \) is the unit mass, \( N_s \) is the number of particles impacting to the wall.

All solutions obtained from DSMC are unsteady. Statistics of these results taken over a large amount of time produces the steady state results. Steady state is assumed to be reached after a certain time passes. Generally, to determine the amount of time required for reaching steady state, the total length of the domain is divided by the molecular speed. It is important to note that the molecular speed includes both thermal speed and mean flow speed.

For classical DSMC, the mean flow speed is specified as it is the inlet boundary condition. On the other hand, for pressure driven flows, this poses another difficulty since the mean flow speed is a quantity that can be obtained from the flow field which the
result of the problem to be solved. For pressure-driven flows, therefore, an estimated value of mean flow speed must be used to initiate the particles. This value should not have any effect on the results as it will be forgotten.

Alternative methods for determining steady state convergence may include recording the changes in physical flow quantities such as pressures or densities at consecutive runs. However, since the statistical fluctuations are large with the DSMC method, it is difficult to determine when the steady state convergence occurs.

The DSMC procedures described above are then repeated a sufficient number of times. Pre-determined time intervals can be given between two successive sampling processes since the sampled data are not used in any other part of the DSMC method other than writing the restart and output files.
CHAPTER TWO: LITERATURE SURVEY

In the past years, with the developments in microsystems, an increasing effort has been made to understand and predict the flow properties in micro geometries. Based on a number of theoretical, computational efforts and also experimental studies, it is now obvious that the transport mechanism in microscale devices differ than those in larger systems.

These studies have shown that the load capacities of microbearings diminish, the electric currents required to move micromotors is extraordinarily high, some liquid flows may choke in the channels, the dynamic response of micromachined accelerometers at atmospheric conditions is overdamped, the pressure gradient in a long microduct is not constant, and velocity slip and temperature jump can no longer be neglected at the solid boundaries.

Some common explanations attributed to the terms neglected in macro theory and gain importance in microscale where the surface area to volume ratio is very high. This may substantially increase surface forces acting on the flow and affect mass, momentum and energy transport causing nonlinear changes in thermodynamic fluid properties such as viscosity. For instance, viscosity is usually assumed being independent of the channel dimensions. On the other hand, there are some observations showing that this is not a valid assumption for various liquids.
As the mean free path of the molecules approaches to the order of the system size, the molecules become more closely packed at normal pressures and temperatures. As a result, attractive or cohesive potential between the molecules as well as the thermal and momentum accommodation coefficients of the surface become dominant parameters describing the flow. For macro channels, the friction coefficient generally decreases with increasing height to width ratio. On the other hand, measured flow rates are found sometimes higher and sometimes lower than predicted by continuum models. In other words, the friction factors unpredictably differ from the theoretical predictions in micro channels.

Furthermore, many microfluidic devices cannot be characterized by either a simple laminar or turbulent model, because the length of the element in the direction of flow is shorter than the entrance length. Actually some of the researchers like Peng et al (1995) suggested newer correlations relating friction factors to Reynolds number as microscale effects are visible at low aspect ratio and low Reynolds numbers for certain liquids.

Along with all these theoretical concerns, many questions regarding the practical side that may expectedly affect flow behavior remain unanswered.
Although none of them has not been proven yet, the nature of fluid, surface roughness of microchannels, imperfections on the channel walls that may come out during manufacturing process, incapabilities of available experimental procedure, apparatus and uncertainties related to measurement techniques and processes are some of the common answers.

With the help of kinetic gas theory and molecular based models, the literature of gas flow in microchannels is relatively more developed compared to that of the liquid flow. Although it is possible to find microscale studies in the literature involving with a variety of gases, there is still lack of information. In addition to this deficiency, the results of the earlier studies in this field are not consistent and they mostly disagree with each other.

**DSMC Studies**

The numerical DSMC method has been successfully applied for hypersonic or rarefied gas flow studies since Bird (1976, 1994) participated in the development of the model. Recently, the method has also been used in several novel applications in the physics and chemistry such as nonequilibrium fluctuations, dense gas dynamics, micro and nanoscale flows, and surface studies involving liquid-vapor and surface interface.
The theoretical background of DSMC as well as comparison with molecular dynamics and the other available methods are reviewed by Bird (1978). Some of the other comprehensive reviews in the field are done by Muntz (1989), Cheng (1993), Cheng & Emmanuel (1995) and Oran et al (1998).

The DSMC studies investigating the structure of the shockwaves in rarefied monatomic gases are summarized and compared by Muntz (1989) and Muntz et al (1989) highlighting the computational aspects of the DSMC method.

Other than simple numerical density calculation tests done by on normal shock structures in high Kn in the range of Mach 5-10, Erwin et al (1991) measured highly non-equilibrium velocities inside a hypersonic normal shock wave in helium at Mach 25 and compared the results with DSMC calculations. The DSMC was quantitatively able to capture the features of these experiments.

More complex studies such as of Bird (1987) and Moss et al (1988) used complicated chemical and radiation transport for a normal shock configuration in air with a 10 km/s shock. The comparisons in equilibrium and un-equilibrium regions are captured well by the method and the results are used to refine chemical model. A further study has been done to study the flow around spacecraft as well as plume impingements on satellites.
The other studies in hypersonic viscous flows and high-temperature gas dynamics are reviewed by Cheng (1993) emphasizing the important and practical aerospace applications.

Curtis (1994) used the DSMC to investigate a spacecraft aerobraking during the entrance to a planetary atmosphere. A 3-D flow simulation of reentry capsule is done by Ivanov et al (1997) considering the nonequilibrium molecular interactions at a typical range of altitude. Various angles of attack are used and the results are compared with the experimental data available.

Cheng and Emmanuel (1995) compared DSMC with Navier-Stokes and experiments for in the low Kn regime.

Oran et al (1998) reviewed the background, principles, advances and a number of other applications of DSMC, and provided with a comprehensive literature search in an excellent review article. An overview of the use of DSMC to simulate important applications of transitional and nonequilibrium flows is given. Selected new and potentially important advances in DSMC capabilities are described and future directions in the method are discussed.

Film growth and plasma etching are two crucial processes in today’s silicon and semiconductor industry. The conditions in the chamber must be controlled precisely to
achieve small feature size and consistent production. In application of these techniques, most of the time low pressures and low densities are involved and desired for a better control of the process. Hence, the DSMC becomes suitable for the modeling purposes.

A recent work that uses DSMC as a basis for modeling CVD is done by Coronell and Jensen (1992, 1993). It has been shown that although the surface diffusion is not very important for covering a step with films made of metal and refractory materials, it affects the surface roughness.

A recent work for plasma etching simulation by Johannes et al (1996) modeled a high-density chemically reacting commercial plasma-etch system at low pressures by employing a DSMC code to describe the neutral and ion transport.

Furthermore, studies by Muntz (1989), Cheng (1993) have also shown that the solutions of the DSMC method in the limit of very low Kn approach the solutions of the Navier-Stokes. Likewise, Morris et al (1992) showed comparisons of DSMC with molecular dynamics are in excellent agreement in slip lengths.

The classical DSMC algorithm uses rectilinear, orthogonal and Cartesian grid which are the most cost-effective ones. However, any type of cell structure can be employed as long as the particle addresses can be determined during the simulation.

Hence, to expand the scope of DSMC, variable cell sizes, sophisticated body fitted, and gradient related adaptive cells have started been utilized in the DSMC calculations Ivanov et al (1997), Cybyk et al (1995). It is shown that in more accurate solutions are obtained the high-gradient regions although the solution takes longer time than it would take with classical DSMC with the same number of computational cells.

Parallelization of the DSMC codes efficiently has become the main focus of the recent relevant studies to speed the DSMC processes up. Especially, sorting and indexing subroutines require intensive interprocessor communication and take the longest time in the whole procedure. Also processor-load balancing should be optimized to carry out pair collisions. Oh (1996) has found that the parallel efficiency of DSMC is 10%-20% less than one would obtain for continuum CFD codes.
Despite the challenges encountered in advancing the code’s efficiency, all of these earlier attempts helped the DSMC develop as an attractive computational tool when simulating realistic high speed flows with high Kn numbers.

**DSMC on Micro Flow**

With the advent of MEMS technologies, researchers have turned their attention to microflows characterized by high Kn. The natural instinct was scaling down the computational domain of a proven method, the classical DSMC.

However, some of earlier attempts using DSMC to simulate microchannels including Oh (1995), Ahn et al, (1996), Piekos and Breuer (1996) have brought serious questions about the applicability of DSMC to low speed microchannels because of the theoretical and computational difficulties inherent in the method.

The standard DSMC was originally designed for high-Ma flows with constant inlet velocity and vacuum outflow boundary conditions. Certainly, driving any gas with a Ma number of 4 or 5 through a channel with a height of 0.4 µm is not realistic. Using constant inlet velocity is physically impractical. Furthermore, using the vacuum boundary condition at the exit boundary where no molecules enter the domain is inappropriate. Especially for subsonic flows where thermal motion is of the same order of magnitude as the mean flow, such a boundary treatment is unrealistic.
To induce correct propagation of information across the boundaries, there should be a substantial amount of backpressure allowing the particles to come inside from the outlet boundary as well.

Nevertheless, it is very common to find the DSMC studies on micro-flow geometries having hypersonic flows with these impractical and unrealistic boundary conditions. In the later sections of the study, these problems and other difficulties will be explained more in detail.

The developments over the classic algorithm of Bird (1994) include different algorithms accounting the particle collisions, and treating wall and outlet boundary conditions. Ikegawa and Kobayashi (1989) computed streamwise inlet velocity from the total particle flux. Another important step was taken by Nance et al (1997) by imposing a pressure boundary conditions based on theory of characteristics at the exit plane. This method gave satisfactory results for microflows compared to those obtained by Piekos and Breuer (1996) with particle-counting.

Garcia et al (1997) has summarized some of their recent studies in which the DSMC method has applied to a few novel applications such as surface dynamics studies, hydrodynamic and chemical fluctuations, and liquid-vapor dynamics.
First, the DSMC method is used to simulate a computer disk drive consisting of a head and a rotating platter. In reality, the disk head floats less than 50 nm above the spinning platter. Knudsen number for this geometry is of order unity. Having the dilute gas layer occupying the space between the head and platter, the system forms a slider air bearing. The pressure along vertical direction is also taken to be constant. The surface temperatures are assumed to be constant at 273 K. At the left and right boundaries the gas pressure is fixed at ambient pressure. To maintain ambient pressure at the inlet and outlet, the flow velocities are adjusted according to the ambient density and temperature.

For the simulation, two horizontal plates having a length of 5 µm are placed 50 nm apart. The lower plate moves with a velocity of 25 m/s. The number of simulation particles is 16,000. The accommodation coefficient is selected either 0.9 or 1 for Cercignani-Lampis-Lord surface scattering model. At these conditions Knudsen number is of order unity.

To validate the results, the resulting pressure distribution is compared with the results of Reynolds equation with slip correction and a more sophisticated formulation by Fukui and Kaneko (1988). A good agreement between DSMC and Fukui-Kaneko theory is obtained.

In the second part of the study, the hydrodynamic and chemical fluctuations have been investigated. For the study that involves investigating the hydrodynamic fluctuations in a one-dimensional system, two stationary horizontal plates at different temperatures
separated by a distance are considered. The separation distance is chosen as 50 times of the molecular mean free path. The results are found to be in good agreement with numerical solution of fluctuating hydrodynamic equations for the given temperature ratio. Also, the method has been applied to a similar system under a constant shear where the wall velocity is about twice the sound speed. And the results were found to be matching with their molecular dynamics simulations. This study is left for the future work to be extended to fluctuations near hydrodynamic instabilities.

Next, the fluctuations in a dilute gas with chemical reactions are considered. A random fraction of collisions is taken to be reactive. A homogenous system in which the chemical system has a bifurcation of its steady state and a spatially extended chemical system are considered. It has been shown that DSMC simulation is in excellent agreement with the numerical solutions used for comparison.

In the final part of the study, the DSMC method is used to calculate thermal properties of a moderately dense non-ideal gas. The Boltzmann equation, its expansion Chapman-Enskog, and even the standard DSMC which is equivalent to solving Boltzmann, all contain an inconsistency that is calculating the transport properties of a dilute gas of hard spheres assuming an ideal gas equation of state.

Although modified collision rates introduced by Bird (1994) to reproduce the transport properties of the non-hard sphere gases, these modifications retain in the ideal gas
assumption. Therefore, the collision step has been modified to include extra separating that hard sphere particles would experience after a collision.

Moreover, Enskog Y-factor is employed to calculate the probability of a collision due to the volume occupied by the spheres. Having this density dependent collisions and variable displacement the new method is called the CBA (Consistent Boltzmann Algorithm). It would not be wrong to say CBA and Enskog simulation Monte Carlo have removed the DSMC’s limitation to dilute gas. A Mach 2 shock wave in shock tube having a length of 70 times of the mean free path is used for different number densities. The transport coefficients numerically determined using CBA, those derived with analytically from the kinetic theory, and obtained with MD simulations are found to be in good agreement up to moderate densities.

The same method is recently applied to subsonic nonideal gas flow and heat transfer in micro and nanochannels by Wang and Li (2003). To incorporate non-ideal gas effects, the Van der Waals equation is used to describe the equation of state. The Enskog theory for dense gases is used to modify collision rate. The constant inlet velocity and vacuum conditions are used to simulate gas flow. Different inlet Knudsen numbers ranging from 0.05-1 are studied in short microchannels having an aspect ratio of 5. The results showed that the non-ideal gas effects become significant as the gas density increases and as the channel height decreases. A substantial amount of decrease in the skin coefficient and a different heat flux mechanism at the wall are observed.
In a recent study done by Pan et al (2000) the DSMC algorithm is modified to reduce the statistical scatter by splitting the random velocity, temperature and stress tensor into two parts. The method is used for the study and simulation of the stationary gas and low-speed micro Couette flow with infinite plates where there is no temperature gradient in the flow. A sample size of $3.2 \times 10^6$ is used for obtaining the results. This method requires an additional computational effort and consecutive executions of the code with adjustments of slip velocity obtained from the previous run. However, less statistical noise is obtained through this method.

Pan et al (2001) later on introduced a number of big molecules in the flow to replace the real molecules since the statistical scatter is less for molecules having larger mass. In this method, as in Pan (2000), the reference diameters of the particles are adjusted keeping the mean free path and dynamic viscosity the same. The time step and the number of collisions are also modified accordingly taking the change in the molecular mass into account.

The method is applied to micro Couette and plane Poiseuille flows. At a sample size of $2 \times 10^6$, the results generally showed good agreement with slip flow theory and classical DSMC results with small discrepancies.
The DSMC method has been applied to various micro geometries with additional improvements such as in Fang and Liou (2002). However, there is a need for future investigations of general flows in microchannels with improved DSMC based algorithms.
CHAPTER THREE: PROBLEM STATEMENT

The internal cooling of turbine blades is essentially crucial as the temperatures associated in typical gas turbine engines is close or even beyond the melting point of the blade material. The temperature level and variation within the blade must be controlled for increasing longevity and durability of the blades.

Rib Turbulators

Film Cooling

Cooling Passages

Trailing

Edge Ejection

Figure 5. A turbine blade with rib turbulators

Rib turbulators which can be square or rectangular are generally placed on opposite walls of the coolant passage. Symmetric or staggered arrangements can be done. Using rib turbulators inside the blades increases the internal convective heat transfer coefficients and thereby helps turbine blades cool by disturbing the near-wall flow. The flow pattern created by the ribbed channel is one of the major factors determining the cooling effectiveness. In order to make more informed decisions about the blade designs, the flow pattern and the heat transfer characteristics inside turbine blades must be fully understood.
Extensive research has been conducted on various aspects of the rib-roughened channels and it is concluded that the degree of local and overall heat transfer enhancement depends upon the passage aspect ratio, rib height to passage hydraulic diameter or blockage ratio, size, shape and placement of the rib turbulators, angle of attack, and Reynolds number. Interested readers can refer to the articles by Webb et al (1971), Han (1984), Han et al (1985, 1992), Chandra and Han (1989), Taslim et al (1991), and Zhang et al (1994). The recent developments in turbine blade internal cooling are reviewed by Han and Dutta (2001).

This geometry has also practical importance in the integrated circuit design and packaging since flow and solid surface temperatures can be chosen independently.

Very few researchers have investigated the effects of Kn and different wall temperatures on the heat transfer mechanism in microchannels. The heat transfer is typically considered negligible when the wall is isothermal and at the same temperature as the
flow. However, the incapability of continuum methods and expensive computations with particle methods in this regime should not be the reason or explanation to take that assumption without any investigation.

Ultimately, the flow features inside the channel will be different and the assumption will not be valid when cooling or heating exist due to a different wall temperature. Therefore, the main aim of this study is to develop and apply the Information Preservation (IP) solution algorithm over the classical DSMC method with the implicit pressure boundary conditions.

The general applicability of the method in solving a real flow situation will be verified using the backward facing step flow simulation. There are numerous investigations involving turbulent incompressible flows over the backward facing step which has emerged as prototype one a nontrivial yet simple geometry. The computations to understand both instability and transition to turbulence help expand the database for this benchmark problem. The review paper of Eaton and Johnston (1981) includes earlier references in the field.

Nevertheless, even for the incompressible fluid cases, there are only a limited number of studies to refer such as Armaly et al (1983), Barton (1997), Tangham and Knight (1989) when the Reynolds number is less than 400. Very recently, Biswas et al (2004)
investigated 2D and 3D backward facing step flow for various expansion ratios at low and moderate Reynolds numbers.

Despite theoretical and practical importance, the lack of studies involving laminar gas flow over backward facing step geometry is evident. Moreover, considering the microscale fluid behavior differs from the macroscopic predictions, thorough investigation of low-speed gas flows over backward facing steps in microchannels is needed for proper design and thermal management of MEMS.

**Numerical Simulation**

The following figure presents the backward facing step geometry in a microchannel with nitrogen gas as the working fluid. The channel dimensions are 2.0 µm in length and 0.4 µm in height. The backward facing step covers half of the channel height at the entrance and it extends up to 1/8th of the channel starting from the left inlet boundary. Nitrogen enters the channel at 300 K in all of the cases studied. The channel initially is filled with gas based on the inlet temperature and pressure conditions. The upper and lower walls as well as step surface are all diffusively reflective and kept at 323 K.

The 2-D computational grid consists of uniform rectangular cells. The total computational time is directly proportional to the number of simulated particles used in the simulation. The usual practice is using around 20 particles per cell in standard DSMC
calculations to obtain results with less statistical scatter. In our calculations, the number of particles is kept at a minimum of 50 per cell.

**Benchmark Problem**

For benchmarking the algorithm in a geometrically simpler simulation, two parallel plates are placed in a rectangular 2-D computational domain whose dimensions are 0.4 µm by 2 µm. The aspect ratio of the simulated microchannel is 5 which is lower than those usually found in experiments. The plates are diffusely reflective and located at the upper and lower boundaries of the domain fully covering the top and bottom boundaries. Nitrogen gas will be used as the working fluid. Constant pressures of 2.5 atm and 1.0 atm are assigned for the inlet and outlet stream boundaries respectively. Only the inlet flow temperature is specified as 273 K and outlet temperature will be determined according to the conditions inside the channel. The initial state in the channel is set by the density requirements that can be obtained from the inlet pressure and temperature.
Figure 8. Sample problem flow geometry

The initial state is determined by the density requirements.

Stationary diffuse plates lay on the top and the bottom boundaries.
CHAPTER FOUR: COMPUTATIONAL APPROACH

Numerical Difficulties with DSMC

Numerical solutions for the explicit continuum methods are limited with strict cell size, and time step requirements. Further limitations apply to stability and accuracy conditions when chemical reactions, molecular diffusion, thermal conduction take place in the numerical simulation. On the other hand, DSMC simulations do not face any of these stability problems that are inherent in the Navier-Stokes solutions.

The computational errors associated with the DSMC are generally caused by the finite cell size, time step in physical domain and the number of simulated particles. Generally, these precision errors become smaller with a smaller time step and a large number of cells.

Inadequacies in the implementation of the physical models involving molecular collision, boundary conditions and gas-solid interactions can be other possible source of errors.

Additionally, the round-off errors exist in numerical computations such as in distributing and tracking particles in space, determining molecular velocities, enforcing boundary conditions and in sampling macroscopic quantities from the microscopic information. In this study, double precision accuracy is employed for handling and storing of variables
instead of 8-digit real number accuracy used in the standard DSMC. It is determined that serious problems occur for the fine cell networks if the standard accuracy is used.

Due to statistical treatment of the intermolecular collisions, the DSMC method deals with a statistical error which is inversely proportional to the square root of the number of simulated particles. Reducing this scatter can be achieved by increasing the total number of simulated particles or sample size. However, recent studies (Pan et al 2000) have shown that there is a limit to this reduction.

Since the computational time depends on the number of particles used in the simulation increasing the number of particles would cause a major problem for the standard DSMC method. On the other hand, using less number of simulated particles may lead to loss of accuracy due to statistical scatter.

The sampling of macroscopic flow quantities from microscopic molecular information is an intrinsic scatter of DSMC due to representing extremely large number of real molecules by a small number of simulated particles.

Further statistical fluctuations occur when mean flow speed is much less than the thermal speed. To explain why DSMC fails when directly applied to the MEMS devices involving low flow velocities, the microchannel used by Pong et al (1994) can be considered. Helium gas at 1 atm and 298 K is used in a microchannel with a height of 1.2
µm, a width of 5 µm and a length of 3000 µm. The Kn is in the range of 0.13 and the inlet flow velocity is 0.2 m/s approximately. The DSMC method seems to be theoretically applicable for these conditions.

The number density of the molecules is relatively high at this pressure. The mean collision time is calculated to be $10^{-10}$ s. To reach the steady state, particles moving with an average velocity of 0.2 m/s of must pass through the channel. This requires a minimum of $1.5 \times 10^8$ time steps since the computational time step must be smaller than the mean collision time in order for DSMC to produce meaningful results.

Unfortunately the problem does not end here since the DSMC starts sampling the macroscopic flow quantities after the flow reaches the steady state. Therefore, the DSMC needs an additional amount of time to produce statistically meaningful results. As it will be explained in detail later, the DSMC faces an unbearable statistical scatter problem for low-speed flows. For the given problem, for example, if a sampling size of $1.5 \times 10^8$ particles per cell is used, the statistical error reduces to 0.2 m/s which is the mean flow speed. This means the DSMC results may involve with a hundred percent error even with such a large number of simulated particles. The computational effort needed to solve such a problem is obviously beyond the current computer resources.

Another difficulty results from the cell size limitation. In the DSMC method, the linear dimension of cells must be smaller than the mean free path. This limitation guarantees
that simulated particles would not jump over a cell without entering it during a given time step. According to the calculations for the specified conditions in the study (Pong, 1994) more than 250,000 cells are required. Considering that each cell should contain a minimum of 20 simulated particles, a total of $5 \times 10^6$ particles are required. This type of a simulation would not be practical to be handled with the currently available computer resources.

The DSMC faces another problem when external boundary conditions are desired to be applied. In the standard algorithm, the classical boundary conditions are the free stream with constant velocity at the inlet and a vacuum condition which discards the particles at the outlet. However, for subsonic gas flows since there must be a substantial amount of backpressure allowing the molecules come inside from the outlet boundary. Therefore, the typical boundary conditions of DSMC are not physically correct for subsonic flows. Liou and Fang (2000) applied implicit boundary conditions for Couette and plane Poiseuille flow problems using a large number of particles. However, the statistical fluctuations in the boundary cells cause problems for standard DSMC when sampling and imposing boundary conditions properly.

Additionally, in the standard DSMC algorithm, there is no limitation in the particle density since the particles can move independently of each other in a time step. Therefore, unrealistic high densities maybe obtained in some cells.
The DSMC has a lot of potential and has already given both qualitative and quantitative answers to a broad range of problems with its simplicity and flexibility. However, difficulties discussed have to be considered and essentially answered if possible in order to get meaningful results out of the classical DSMC method for the microchannel flows.

Although the DSMC method works efficiently for hypersonic and rarefied gas flows, it is difficult to obtain noise-free results with DSMC if the mean flow velocity is much smaller than the random thermal velocity.

Theoretically, in order to reduce the large statistical fluctuations at these low velocities, an extremely large sample size must be used. For instance, the random thermal velocity of a particle simulated in the 2-D DSMC method is calculated as

$$ V_{th} = \sqrt{2RT} $$  \hspace{1cm} (16)

where R is the gas constant, T is the gas temperature. From this calculation, the thermal speed is found to be approximately 395 m/s for air at standard temperature. The statistical theory says that when all the samples are statistically independent, the scatter becomes

$$ \text{Scatter} \approx \sqrt{\frac{2RT}{N}} $$  \hspace{1cm} (17)
where $N$ is the sample size or number of particles per cell. This means that the statistical error tends to zero as the sample number increases.

Theoretically considering a pure random process, to reduce the scatter to order of 1 m/s a sample size of $1.56 \times 10^5$ is required for air at standard conditions. If the number of samples is increased to $1.56 \times 10^7$ the scatter then reduces to 0.1 m/s. A scatter of this size obviously is not a significant error for supersonic flows where DSMC works perfectly. However, the MEMS devices generally involve with gas flows at very low speeds for which these errors can not be neglected. Therefore, obtaining accurate results from DSMC for microflows becomes very expensive.

Unfortunately, the problem is not just the high computational cost resulting from the large sample sizes. The theoretical predictions are valid only for the gases at the equilibrium state. In addition, the processes in the computer simulation can not be completely randomized as the theory requires. Therefore, the particles and the samples can not be statistically independent. To help increase the independency of particles, several time steps are usually given between two consecutive sampling steps. Nevertheless, the tendency of the actual statistical scatter of DSMC may not be the same as predicted by the theory. The magnitude of the statistical error may not decay to zero even for the simulations going beyond $10^8$ samples.
In fact, a sample calculation is performed by Pan et al (2000) for a stationary gas and for a Couette flow geometry using different gases, such as helium, argon, and xenon shows that the stationary gas simulation has an error about 0.02 m/s even with a sample size of $10^9$.

The Couette flow simulation involves with larger statistical errors than that due to the additional effects of a macro motion over a pure random process. However, the findings showed that, although the decrease is not as large as predicted, the error decreases with increasing sample size as the number of samples increases from $3.2 \times 10^6$ to $3.2 \times 10^7$.

However, it is interesting to see that the error increases when the sample size increases to $10^8$. This shows the behavior of statistical scatter of the DSMC does not agree well with the theoretical predictions.

Having characteristic sizes in the order of micrometers, MEMS devices often operate at low or moderate Mach numbers. Therefore, MEMS flow simulation with DSMC method becomes impractical with the current computer resources.
Principles of IP

To address this issue, Fan et al (2001) proposed an information preservation (IP) technique. In this method, microscopic particle velocity can be divided into two parts as

\[ c = V_0 + V_{th} \]  

(18)

where, \( V_{th} \) is the random thermal molecular velocity and \( V_0 \) is the mean flow velocity.

As in the regular DSMC procedure, microscopic particle velocities are used to determine the molecular positions and carrying the molecular collisions out. The information velocity, however, is a macroscopic velocity used to represent the collective flow of a large number of real gas molecules.

In the beginning of the simulation, the information velocity of a particle is set equal to the microscopic velocity of that particle. Once the molecule goes through a collision either with another molecule or with a solid surface the IP velocity is updated. In case of an intermolecular collision, the IP velocity is calculated as

\[ V = V_0 + V_{th}^{\prime} \]  

(19)

where double quotation mark denotes post-collision thermal velocity of the particle.
The post-collision thermal velocities are computed by the IP collision models which will be explained later on. In case of a molecule-solid surface collision, the wall reflection model determines the information velocity for the reflected particle. For instance, in diffuse wall reflection model, the IP velocity of a reflected particle becomes equal to the velocity of the solid surface. Different surface models can easily be employed instead of the diffuse model.

The preserved information of the particles is modified using the pressure field in the modification step using inviscid fluid mechanics equations.

After steady state is assumed, sampling the preserved macroscopic information produces macroscopic mean flow velocity, shear stress and other macroscopic quantities with less statistical scatter since the randomness of the thermal velocity is removed.

Fan et al (2001) showed the IP technique was highly effective in reducing the statistical scatter to simulate Couette, Poiseuille and Rayleigh flows. It has also been shown that even though the computational cost increased due to additional CPU and memory requirements, the computational time is reduced vastly due to less number of samples. Cai (2000) has then modified the method and applied it for two dimensional micro-scale flow by utilizing the continuity equation in determining the flow field.
Fan et al (2001) used a simple molecular collision model which is developed for a constant density system. Furthermore, to work with IP, the molecular diameters are modified based on the available experimental data. By affecting all calculations in the simulation this may produce incorrect results.

Another important shortcoming of both of these studies is the assumption of the isothermal flow. In other words, the molecular temperatures are assumed to be equal after collisions. This assumption can be valid only if the speeds involved are very low and the flow boundaries are at the same temperature as the flow.

Sun and Boyd (2002) then modified and developed an IP algorithm for general flows where the macroscopic temperature is also preserved in DSMC particles. The steady or low frequency unsteady flow modeling through IP is successfully validated in this study. Considering continuum flows, it is known that the velocity and temperature of the flow does not only depend on momentum and energy exchange but also on the pressure field. Therefore, inviscid fluid mechanics equations in Lagrangian description are used to modify and update macroscopic velocities and temperatures at the end of each time step.

An additional temperature or energy concept is used by Sun and Boyd (2002) since there is a difference between the volume-averaged translational energy of a particle and the average translational energy if the particle passes an interface, i.e. a cell boundary. In
order to satisfy energy conservation, these additional energies in form of temperatures are needed to be evaluated for calculating the molecular and average cell temperatures.

The calculation of additional temperature is done as follows. First, the interface temperature is calculated through interpolation using the temperature of the cell that the particle exits and the cell that the particle enters. This temperature is also called reference temperature. The energy of a fictitious particle at a temperature of $T^*$ moving opposite direction passing through the same interface is then calculated using the Boltzmann constant and the difference between the particle temperature and the reference temperature.

Sun and Boyd (2002) investigated macro-scale Couette and Rayleigh flows as well as flow over a NACA airfoil. In Couette flow problems, infinitely long plates and domain used with a separation of one meter. For plates moving at opposite direction at 1 m/s, at a Knudsen number of 1, the results showed that IP predicts the velocity field very satisfactorily with $10^4$ particles per cell. On the other hand, the theoretical prediction of the velocity scatter is 0.2 m/s with DSMC method with a sampling size of $10^8$.

For another Couette flow case with 200 cells in calculation domain, the DSMC needed 100,000 sampling particles per cell while IP needed only 1,000 per cell for Kn=0.01 and 10,000 particles for Kn=100. To compare and validate IP results there are two additional DSMC results in the study with 20,000,000 samplings each.
The performance of the IP method in eliminating the statistical scatter is validated for simpler microscale gas flow simulations where local thermal equilibrium is believed to be established. Therefore, in this study, the IP algorithm of Sun and Boyd (2002) is chosen to be built over the classical DSMC algorithm of Bird (1994).

Since the algorithm of Sun and Boyd (2002) works in unidirectional flows, simulation of a 2-D parallel plate microchannel flow with a specified channel length is not possible. Furthermore, the standard DSMC boundary conditions, i.e. constant inlet velocity and vacuum outlet boundary conditions are applied.

In the present study, this algorithm is adapted to simulate a 2-D short microchannel flow with implicit pressure boundary conditions. The final algorithm is first benchmarked with a plane Poiseuille flow. Then, the gas flow and heat transfer mechanisms over backward-facing step in short microchannels in transition regime is investigated.

**How IP Works**

In the IP method, there are five additional variables that each particle carries besides the variables of classical DSMC method. These include 3-dimensional macroscopic velocity vector, macroscopic temperature, and additional macroscopic temperature.
Additionally, average macroscopic velocity, temperature, additional cell temperature, pressure, and density are calculated for each cell to update the particle information.

All additional temperatures are set to zero initially for those already inside and for those entering the domain at any time. The initial and boundary conditions are used to determine the initial values of the other variables.

The particle velocity is defined as the linear combination of the mean flow speed and random thermal velocity. The particles inside the flow domain and the new particles entering the domain all have this total velocity. At the inlet, the thermal velocity is obtained using the inlet temperature which is always constant. However, if pressure boundary conditions are specified, the temperature at the exit plane varies with time.

The particles move in the domain with their velocity defined and controlled by the regular DSMC procedures. When a particle collides with another particle for the first time, the post-collision velocities are determined using the molecular thermal velocities. Then, the macroscopic particle velocity is calculated adding the guessed value of the mean flow velocity onto these post-collision velocities. From this point, these macroscopic velocities are preserved and used for the rest of the calculations.

As mentioned earlier, the simple collision method suggested by Fan (2001) is incapable of calculating gas viscosity successfully. Fan (2001) simply set the post collision
velocities of particles equal to each other after the collision. Since this algorithm is isothermal or too simple the thermal effects cannot be modeled correctly.

Sun and Boyd (2002) has tried to develop a new, improved algorithm for computing post collision velocities of the colliding particles. In this model, the post-collision states of the collision partners are different than each other. A post-collision deflection angle concept is also tried to be incorporated by Sun and Boyd (2002) in determining the post-collision velocity and temperatures. However, since the deflection angle is defined in terms of pre- and post- collision velocities, the problem becomes a 6-equation non-linear system.

The numerical solutions developed in the present study for sample calculations showed that the cosine of deflection angle that is used in the calculations turned out to be always equal to 1. An analytical investigation proved that this is the case.

Therefore, in the present study, the post-collision quantities are simplified by omitting the unnecessary deflection angle calculation. This saves a significant amount of computational time since the collision routine is a part of the simulation that is repeated numerous times for each and every time step.
The simplified post-collision quantities are calculated as follows

\[ V_1' = \frac{1 + C_\mu}{2} V_1 + \frac{1 - C_\mu}{2} V_2 \]  
(20)

\[ V_2' = \frac{1 - C_\mu}{2} V_1 + \frac{1 + C_\mu}{2} V_2 \]  
(21)

\[ T_1' = \frac{1 + C_\kappa}{2} T_1 + \frac{1 - C_\kappa}{2} T_2 + \frac{(V_1 - V_2)^2 (1 - C_\mu^2)}{4 \zeta R} \]  
(22)

\[ T_2' = \frac{1 - C_\kappa}{2} T_1 + \frac{1 + C_\kappa}{2} T_2 + \frac{(V_1 - V_2)^2 (1 - C_\mu^2)}{4 \zeta R} \]  
(23)

where \( V_1 \) and \( V_2 \) are pre-collision velocities, \( T_1 \) and \( T_2 \) are pre-collision temperatures, \( C_\kappa \) and \( C_\mu \) are numerically determined coefficients, \( \zeta \) is the number of degrees of freedom, \( R \) is gas constant. These coefficients are numerically determined by Sun and Boyd (2002) for five different gases (\( N_2, \ O_2, \ He, \ Ar, \) and air). The numerical results of low-speed macro Couette flow simulations are compared with the shear stress calculations from the analytical solution and heat flux calculations from the numerical DSMC calculations. The simulations are done at a Knudsen number of 0.01 based on the VHS model. Comparison with the experimental studies also confirmed that these coefficients are constants.
In order to conserve the energy of the system, the IP method requires additional temperature values both for molecules and computation cells. The molecules exiting a cell borrows an additional energy from all other molecules remaining in that cell in the amount of \( ak(T_i - T_{ref}) \).

This additional amount stems from the contradiction between the real flux and IP flux model. The translational energy which is carried by an individual particle is \( \frac{3}{2}kT \) according to the kinetic theory of gases. However, when the molecule passes an interface the average translational energy transferred between the two medium becomes \( 2kT \). In stationary equilibrium, the net energy effect is zero assuming the number of particles is uniform in all directions. On the other hand, this energy cannot be balanced for inequilibrium flows automatically.

For steady flows with low mean flow velocities, for each particle leaving the cell there is another particle entering the cell either from the same or another cell interface. If the molecule enters from the same interface, the net energy flux becomes zero. However if the corresponding molecule enters the cell from another interface of the cell, the difference in the transferred energies must be balanced. Therefore, each particle crossing an interface carries an additional energy depending on the interface temperature. This energy is supplied by the other particles in the cell equally to conserve the energy. Since the flow temperatures of the different interfaces of the cell are relatively close to each other, the resulting statistical scatter is very small.
The net energy flux between the cells is then balanced in an average sense. This is an acceptable approach since the aim of the IM method is to preserve the total energy of the system to reduce statistical error, not to restore the microscopic energies.

The additional cell temperatures are used to keep track of these additional molecular energies and distribute them among the particles in the cells. Based on these arguments, for the particle, i, exiting a cell the required additional temperature calculations are done as follows

\[
T'_{i,a} = \frac{T_i - T_{\text{ref}}}{\zeta}
\]

(24)

\[
\Delta T_{c,a} = -\Delta T_{i,a}
\]

(25)

where prime denotes the newly assigned value, subscript a stands for the additional value, c means cell, and \(\Delta\) is the difference between the new and old values of the quantity, \(T_{\text{ref}}\) is reference temperature which is simply calculated at the cell boundary by interpolation.

When a particle strikes to the wall, a similar energy transfer procedure takes place depending on the surface type. First, the velocities are calculated according to the DSMC algorithms explained in the previous sections. Shortly, if the wall is specular, the normal component is reversed whereas tangential component remains the same.
For a diffuse wall, a biased Maxwellian distribution is used to determine post-impact velocities based on the temperature of the wall.

Therefore, for specular wall, the additional temperature calculations are

\[ T_{i,a}' = -T_{i,a} \]  \hspace{1cm} (26)

\[ \Delta T_{e,a} = -\Delta T_{i,a} \]  \hspace{1cm} (27)

For the diffusively reflective wall,

\[ T_{i,a}' = \frac{T_w - T_{\text{ref}}}{\zeta} \]  \hspace{1cm} (28)

\[ \Delta T_{e,a} = T_{i,a} - \frac{T_i - T_{\text{ref}}}{\zeta} \]  \hspace{1cm} (29)

where \( T_{\text{ref}} \) is defined as the temperature of the collision-free gas flow between two parallel plates at different temperatures, \( T_i \) and \( T_w \).
That is,

\[ T_{ref} = \sqrt{T_w \cdot T_i} \]  

(30)

Once all particles are settled, the additional temperatures of the particles are adjusted using

\[ \Delta T_{t,a} = \frac{T_{c,a}}{N_c} \]  

(31)

where \( N_c \) is the number of particles in the cell.

The additional cell temperature can now be set to zero for the calculations to be done in the next time step

\[ T'_{a,c} = 0 \]  

(32)

The IP method modifies and then updates the particle information according to momentum and energy equations assuming the net energy effect due to additional temperatures is zero.
In the modification step, the following equations are solved by finite volume

\[
\frac{\partial (\rho_c V_i)}{\partial t} = -\nabla p \tag{33}
\]

\[
\frac{\partial \left( \frac{1}{2} \rho_c (V_i^2 + \zeta RT) \right)}{\partial t} = -\nabla (p V_c) \tag{34}
\]

where \( t \) is time, \( \rho_c \) is the mass density in cell, \( V_i \) is preserved macroscopic velocity of the particle, \( \zeta \) is number of degrees of freedom, \( R \) is gas constant, \( T \) is molecular temperature, \( V_c \) is sampled macroscopic velocity of the cell at the current time, and \( p \) denotes the cell pressure that can be calculated as

\[
p = \rho_c RT_c. \tag{35}
\]

The next step is for updating the cell information using the following equations

\[
V_c = \frac{\sum_{i=1}^{N_c} V_i}{N_c} \tag{36}
\]
\[ T_c = \frac{\sum_{i=1}^{N_c} (T_i + T_{i,a})}{N_c} \]  

(37)

\[ \Delta \rho_c = -\frac{\Delta t}{A} \int (\rho_c \mathbf{V}_c \cdot \mathbf{n}) dl \]  

(38)

where \( \Delta t \) is time step, \( A \) is the cell area, \( \mathbf{n} \) is the unit normal of the cell interface and integration is evaluated along the cell boundaries.

After steady state is reached, to output the IP results, the sampling of the preserved information in given time intervals is done as follows

\[ V_{c,smp} = \frac{\sum_{i=1}^{N_{TS}} V_{c,i}}{N_{TS}} \]  

(39)

\[ T_{c,smp} = \frac{1}{N_{TS}} \left( \sum_{i=1}^{N_{TS}} T_{c,i} + \frac{1}{\zeta R} \left( \sum_{i=1}^{N_i} \frac{V_{i,d} \cdot V_{i,d}}{N_i} - \left( \sum_{i=1}^{N_i} \frac{V_{i,d}}{N_i} \right) \left( \sum_{i=1}^{N_i} \frac{V_{i,d}}{N_i} \right) \right) \right) \]  

(40)

\[ \rho_{c,smp} = \frac{\sum_{i=1}^{N_{TS}} \rho_{c,i}}{N_{TS}} \]  

(41)
where \( N_{TS} \) is the number of time intervals passes between two consecutive samples, \( N_i \) is the number of molecules inside the cell, \( T_{c,t} \) is the temperature of the cell, and \( V_{i,t} \) is the velocity of the particles inside the cell at the time \( t \).

The normal component of the pressure acting on the wall can be calculated as

\[
p_w = p + \frac{\sum_{i=1}^{N_S} m (v_{i,inc} - v_{i,ref})}{t_s \cdot \Delta A}
\]

(42)

where \( p \) is pressure inside the cell, \( N_S \) is the number of particles striking to the wall, \( v_{inc} \) is the incoming normal velocity, \( v_{ref} \) is the normal velocity of the particle after the reflection, \( t_s \) is time passes during the impact, and the area of wall element is represented by \( \Delta A \).

The tangential component or shear stress calculation is the same as in DSMC method given previously. Neglecting the vibrational mode of energy, the wall heat flux for the IP method is defined in Sun and Boyd (2002) as

\[
q'' = \frac{\sum_{i=1}^{N_S} \left( \frac{1}{2} m V_i^2 + \frac{\zeta}{2} k(T_i + T_{i,d}) \right)_{inc} - \sum_{i=1}^{N_S} \left( \frac{1}{2} m V_i^2 + \frac{\zeta}{2} k(T_i + T_{i,d}) \right)_{ref}}{t_s \cdot \Delta A}
\]

(43)
where $V_i$ is the magnitude of the preserved macroscopic velocity, $k$ is the Boltzmann constant, $T_i$ is the preserved macroscopic temperature, the subscript $a$ stands for the additional information, the superscripts inc and ref correspond to incoming and reflected states respectively.

**Pressure Boundary Conditions**

As mentioned in the previous chapters, the traditional DSMC boundary conditions for supersonic flows i.e. specified number density, constant free-stream velocity and vacuum outlet condition are physically incorrect for microchannel flows. These data are also hard to obtain and control by simple experimental measurements or techniques. Therefore, pressure boundary conditions must be applied.

Generally, inlet temperature and pressure and outlet pressure are known and can be identified as the determining parameters for any flow experiment. In the IP algorithm, these parameters are the initial parameters that the program would ask as inputs. The correct velocity information would be collected from the cells inside the domain once the inflow and outflow conditions propagate into the domain as the simulation continues.

One of the first attempts to model pressure boundary conditions for DSMC algorithm was based on particle conservation. Using the number flux at the boundary, in other words, counting the number of the particles passing the boundary in positive and negative flow
directions in a single time step, the average inlet velocity for the whole boundary or the boundary-cells is calculated. However, particle conversation methods fail for flows with low inlet velocities since the number of particles passing the boundaries is small. This causes large scatter in inlet velocities and therefore makes the solution unstable.

Nance (1997) investigated long microchannels using parallel DSMC. Theory of characteristics for subsonic flow is employed for the first time for DSMC to incorporate pressure boundary conditions at the outlet assuming inviscid and adiabatic conditions. However, at the inlet plane particle flux conservation is applied. Fixing the temperature and transverse velocity component, the streamwise velocity components are updated from the inside the flow field.

An alternative method is proposed by Fang and Liou (2002). Basically, the specified boundary pressure is used to update the flow field at the downstream channel end. The theory of characteristics is utilized with the information inside the domain to calculate velocities and internal energies for the particles entering the physical domain from the downstream boundary. For the upstream boundary, however, the average cell velocities inside the domain are taken as the mean inlet velocities for the boundary cells. However, these velocity values do not carry pressure information and therefore, the time for obtaining stable inlet velocities is large.
While searching an appropriate pressure algorithm for the present study, it is realized that a fundamental mistake is done by Wang and Li (2003). The researchers used several 2-D microchannels having different sizes in order to investigate the similarity of ideal gas flows in micro and macro scales. By changing the inlet number densities, the inlet Knudsen number is tried to be kept constant for all cases. However, while trying to apply external pressure boundary conditions, the problem is overspecified. The inlet temperature, both Kn and Ma at the inlet boundary are specified along with the inlet pressure. This mistake is not realized by the authors. However, only two out of three (pressure, temperature and velocity) can be freely specified at the inlet and only one at the outlet. In the study, the tabulated number densities, therefore, do not correspond to pressures that are supposed to be applied to the inlet boundary. With this mistake, it is concluded that the macro and micro scale flow fields are all identically similar by the Ma and Kn regardless of the channel sizes. The authors noted that the pressure and density plots are different in magnitude although the normalized plots are found to be the exactly the same.

If one would like give boundary conditions in terms of pressure and temperature, the velocity values cannot be known beforehand. The correct velocity information would be collected from the cells inside the domain once the inflow and outflow conditions propagate into the domain as the simulation continues.
In their following study, Wang and Li (2004) implemented the theory of characteristics for the upstream boundary. The inlet number density is calculated using the specified inlet pressure and temperature. The downstream boundary is treated using the same method as Nance (1997) and Fang and Liou (2002). The acceptance-rejection method and Maxwellian distribution are used to determine molecular velocities and the number flux of the molecules entering the computational domain.

However, both Fang and Liou (2002) and Wang and Li (2004) applied a cut-off value to limit the random thermal speed in order to prevent fluctuations at the boundaries. With this treatment the molecular velocity components for entering molecules are also limited.

Utilizing the IP method, in the present study, this treatment is removed allowing the original DSMC procedures decide the molecular velocities without any restriction. The details of the algorithm are given in the following section.

**Upstream Boundary**

The inlet pressure and temperature are specified by the user. Density and speed of sound obtained from the boundary cells inside the domain to calculate average cell inlet velocity for these cells.
Using the characteristic theory which is originally introduced by Whitfield (1984), the three components of the average cell velocities can be written as

\[ (u_{in})_c = u_c + \frac{p_{in} - p_e}{\rho_c a_c} \]  

(44)

\[ (v_{in})_c = v_c \]  

(45)

\[ (\omega_{in})_c = \omega_c \]  

(46)

where the subscript \( c \) denotes average cell values.

The number density, \( n \), is calculated initially using ideal gas law in the inlet cells.

\[ n_{in} = \frac{P_{in}}{kT_{in}} \]  

(47)

Since the gas flow is generally considered in quasi-equilibrium, the Maxwellian equilibrium distribution function can be used to calculate velocities of the entering particles at the inlet and exit boundaries. Noting that the classical DSMC method allows only incoming particles from the inlet domain, the new algorithm has to allow particles come inside the domain from the exit boundary as well.
The Maxwellian equilibrium distribution function, 

\[ F_c = \frac{n_c}{2\sqrt{\pi\beta_c}} \left( \exp\left(-s_c^2 \cos^2 \vartheta\right) + \sqrt{\pi}s_c \cos \vartheta \left[1 + \text{erf}(s_c \cos \vartheta)\right] \right) \]  

(48)

where

\[ s_c = U_c \beta_c \]  

(49)

\[ \beta_c = \frac{1}{\sqrt{2RT_c}} \]  

(50)

use the local average cell velocities and temperatures. Here \( F_c \) represents the number flux through a boundary or a cell. Error function is denoted by erf where \( R \) is constant and \( n_c \) is the number density of the particles in the cell \( c \). The value of \( \vartheta \) is zero for the inlet boundary and \( \pi \) at the downstream exit boundary.

The acceptance-rejection method determines the streamwise velocities of a particle entering the physical domain.
For a cell located at the domain boundary, the remaining velocity components can be written as

\[
\nu = A \cos \phi \tag{51}
\]

\[
\omega = A \sin \phi \tag{52}
\]

where \( R_f \) is a random fraction, \( V_{mp} \) is the local most probable thermal speed of the particle at local temperature. The magnitude, \( A \), having a value between 0 and \( \infty \), can be calculated using acceptance-rejection method.

\[
A = \frac{\sqrt{-\ln(R_f)}}{\beta} = \sqrt{-\ln(R_f)} V_{mp} \tag{53}
\]

\[
\phi = 2\pi R_f \tag{54}
\]

\[
V_{mp} = \sqrt{2RT_c} \tag{55}
\]
**Downstream Boundary**

Using the characteristics theory

\[
(\rho_{ex})_c = \rho_c + \frac{p_{ex} - p_c}{a_c^2} \quad (56)
\]

\[
(u_{ex})_c = u_c + \frac{p_{c} - p_{ex}}{\rho_c a_c} \quad (57)
\]

\[
(v_{ex})_c = v_c \quad (58)
\]

\[
(\omega_{ex})_c = \omega_c \quad (59)
\]

\[
(T_{ex})_c = \frac{P_{ex}}{(\rho_{ex})_c R} \quad (60)
\]

In all of these equations, the cell averaged values, denoted by subscript c, are obtained by simply averaging the molecular quantities inside the cell. And the original acceptance-rejection method in DSMC is kept the same without any modifications.

As the simulation continues, the average cell properties needed are obtained from IP method at every time step. Getting this information accurately is crucial for determining
the properties of the molecules entering the domain. Since the IP method provides the required information with less statistical noise, application of the pressure boundary conditions is practical even for flows with low speeds.

Further Modifications

Generally, for DSMC simulations, the steady state is assumed once the new particles entering from the inlet boundary reaches to the channel outlet. The mean flow speed that is used to initialize the entering molecules is once again used here to determine the number of time steps required for reaching the steady state. Such a mean flow speed can be estimated from previous simulations. As noted before, the final simulation results do not depend on the magnitude of this velocity as it will be forgotten once the simulation starts.

However, a close estimate is useful for a better estimation of the steady state. Because, a premature steady state assumption makes the program spend more time to sample unsteady results. On the other hand, an unnecessarily large estimate of NPS wastes computational time as the sampling of the flow field starts after steady state is reached.

Another important DSMC parameter is the computational time step. The time step must be chosen less the local mean collision time. Since the collision time depends on the mean free path setting an improper time step based on the initial conditions would
produce erroneous results. Therefore, in the present simulation the time step is automatically adjusted during the simulation by checking the maximum distance traveled by the molecules in a given time step. This gives faster results without sacrificing accuracy. Thus, the number of time steps required for reaching the steady state (NPS) is not needed as an input. Automatic determination of steady state again yields the optimal efficiency.

The realization of steady state can also be verified by tracking the macroscopic quantities such as mass flow rate, density or pressure. This concept will be a possible future work as it is not readily built into the current algorithm. However, the simulation results presented here are manually checked for steadiness before steady state is assumed.

The theory limits the linear cell size to the mean free path in order for DSMC to work. This is a physical requirement rather than a stability criterion. As the mean free path increases the number of cells required decreases. This is a clear advantage for parallel plate microscale flow simulations since sometimes a few cells would be adequate to cover the whole channel height.

However, the local mean free path depends on both local pressure and temperature. If the wall temperature is different than the free-stream temperature or if the pressure boundary conditions are employed, the flow temperature at the exit plane changes as the simulation
proceeds. These effects must be taken into account in choosing the cell numbers properly. Hence, generally the cell size is chosen one fourth even one fifth of the mean free path.

For the backward facing step flow case, however, the changes in the local pressure and temperature due to the presence of the step feature make the decision more difficult. Using less number of cells might also prevent predicting the recirculation zone behind the step accurately. Therefore, in our simulations, a minimum of 200 cells are used along the streamwise direction while the number of cells in y direction is varied according to channel height. Obviously, the number of cells can be increased with the expense of the computational cost which depends on the total number of simulated molecules.

As a final note, switching to the double precision accuracy for the spatial variables helped eliminating accuracy problems of the classical DSMC method during determining the molecular addresses for the simulations with very fine cell structures.
CHAPTER FIVE: RESULTS

The Benchmark Problem

The current version of the algorithm is first applied to a Poiseuille flow. This benchmark problem is investigated by Fang and Liou (2002) using the classical DSMC method with implicit boundary conditions.

The height of the microchannel, h, is 0.4 μm, and the length L is 2.0 μm. This aspect ratio of the microchannel is significantly lower than those found in experiments. It is computationally more suitable for DSMC to handle the problem easily.

The inlet flow temperature is 300 K and the wall temperature is set to 323 K. The pressure ratio is 2.5 with an inlet pressure of 2.5 atm.

In the Fang and Liou’s (2002) DSMC approach, the total number of particles is around 180,000. The computational grid consists of 100x60 cells. This gives 30 particles per cell on average. For sampling, a total of 220,000 time steps are used. The steady state is assumed to be reached after 2,000 time steps. The local Kn in the microchannels are found to be varying between 0.055 and 0.123 for these operating conditions.

Although the number of cells in y direction is sufficient, the number of cells in x direction must be higher than 117 according to VHS collision model calculations. This is
an error which is not realized by Fang and Liou. In this study, the number of cells is kept unchanged for a direct comparison. However, our algorithm requires a larger number of particles than standard DSMC. Generally slightly over 50 molecules per cell would be appropriate to carry out simulations without getting any numerical issues. Therefore, for the IP algorithm with pressure boundary conditions, 326,000 simulated particles are used for the current simulation.

Computational time step is dynamically adjusted in the simulation for a better computational efficiency. The steady state is reached around 7000 time steps for the current simulation. Reaching the steady state takes about half an hour on a Windows XP based AMD 64-bit 3500+ personal computer using the Compaq Visual Fortran compiler.

The following figure shows the time evolution of the pressure in a cell located at the one-fourth of the channel and along the centerline. Normalization is done using the value of the exit cell pressure at the current time. It can be seen that the estimated the steady state which occurred at 7,000 time steps is a very good approximation where the normalized pressure reaches a plateau. At given conditions, assuming an early steady state such as before 5,000 time steps would cause spending more computational time in sampling stage as more time would be required to reach asymptotic or steady results.
Figure 9. Time evolution of the normalized pressure in a computational cell located at $x=L/4$ and $y=H/2$

The next figures show temperature and velocity contour plots. As it can be seen, the IP method agrees perfectly well with the DSMC results of Fang and Liou (2002). The advantage of IP over DSMC can be clearly seen through reduction of the statistical noise with in less number of time steps. Although the results presented here are taken after 40,000 time steps, the changes in the sampled flow quantities usually become insignificant after 25,000 time steps.
Figure 10. Comparison of temperature contours a) IP algorithm after 40,000 time steps, b) DSMC solution after 202,000 steps taken from Fang and Liou (2002)
Figure 11. Resulting streamwise velocity profiles with a) the IP algorithm after 40,000 time steps, b) DSMC solution with 202,000 steps taken from Fang and Liou (2002)
To validate the agreement, further comparisons are done using different sampled flow quantities including the heat flux on the walls. For the sake of brevity, the details are omitted in this study. However, to state an example, the wall slip velocity distributions are given in the next figure. The results of Fang and Liou are shown in black with round marks while the current algorithm yielded the distribution shown in blue. A very good agreement is obtained between the results.

Figure 12. Comparison of the slip velocities between the current algorithm and classical DSMC of Fang and Liou (2002)
Before investigating the backward-facing step problem, the variation of the flow speed with channel height can be studied for the same inlet to outlet pressure ratios. This may become useful to evaluate the results of the backward facing step simulation that has four times smaller inlet than the main benchmark problem. Therefore, two additional simulations are prepared with channels having 0.2 μm and 0.1 μm. The channel length is chosen as 2.0 μm for both geometries. The boundary conditions are the same for both configurations. The inlet and outlet pressures are selected as 250 kPa and 100 kPa respectively. The following figure shows the centerline velocity distributions.

Figure 13. Centerline streamwise velocity distributions of channels with smaller flow heights
Expectedly, the mean flow velocity increases as the channel height increases. The difference between two velocity distributions gets larger towards the downstream. Comparing these results with those of benchmark and backward facing step simulations shows that the variation of the velocity with the channel height is consistent.

**Backward Facing Step Flow**

The important parameters of the cases studied in the present study are summarized in Table 3.

<table>
<thead>
<tr>
<th>Case</th>
<th>Cell No in x</th>
<th>Cell No in y</th>
<th>Inlet Pressure (10^5 Pa)</th>
<th>Outlet Pressure (10^5 Pa)</th>
<th>Pressure Ratio</th>
<th>Particles per cell</th>
<th>Inlet Kn</th>
<th>Inlet Density</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>400</td>
<td>40</td>
<td>2.500</td>
<td>1.00</td>
<td>2.5</td>
<td>50.30</td>
<td>0.17</td>
<td>2.808</td>
</tr>
<tr>
<td>2</td>
<td>240</td>
<td>60</td>
<td>1.250</td>
<td>1.00</td>
<td>1.25</td>
<td>55.89</td>
<td>0.34</td>
<td>1.404</td>
</tr>
<tr>
<td>3</td>
<td>200</td>
<td>40</td>
<td>0.375</td>
<td>0.10</td>
<td>3.75</td>
<td>64.67</td>
<td>1.15</td>
<td>0.421</td>
</tr>
<tr>
<td>4</td>
<td>200</td>
<td>40</td>
<td>0.250</td>
<td>0.10</td>
<td>2.50</td>
<td>50.30</td>
<td>1.70</td>
<td>0.281</td>
</tr>
<tr>
<td>5</td>
<td>200</td>
<td>40</td>
<td>0.125</td>
<td>0.10</td>
<td>1.25</td>
<td>60.36</td>
<td>3.47</td>
<td>0.140</td>
</tr>
<tr>
<td>6</td>
<td>200</td>
<td>40</td>
<td>0.125</td>
<td>0.05</td>
<td>2.50</td>
<td>50.30</td>
<td>3.47</td>
<td>0.140</td>
</tr>
</tbody>
</table>

The slip velocity profiles along the lower and upper walls are shown in Figure 12 and 13 respectively. These velocities correspond to the cell-center velocities of the neighboring
cells. As it can be seen, the slip velocities are nonzero and increase towards the downstream due to the decreasing pressure and accelerating flow. As the density drops along the channel with decreasing pressure, the fluid velocity accelerates along the channel.

![Graph showing slip velocity distribution at the lower wall behind the step.](image)

Figure 14. Slip velocity distribution at the lower wall behind the step.

At the section from inlet to one-fifth of the channel the flow acceleration is fast and linear. The increase in velocity does not stop but slows down after that for all cases including Cases 2 and 5. The velocity keeps increasing in a nonlinear fashion till the exit plane. At the exit plane, the slip velocity observes a sudden drop both at lower and upper walls. This particular behavior is not pronounced for the centerline velocity distributions. Nonetheless it is possible to see a small decline for Cases 3, 4 and 6 at the exit plane.
Figure 15. Velocity distribution at the upper wall

It is believed that this drop mainly results from the molecules entering the domain from this boundary towards upstream direction. Nevertheless, a relationship between the amount of the decrease and Kn cannot be formed with limited data. Further investigations are needed to understand the reasons behind this phenomenon occurring at the solid boundaries.

As it can be seen from Figure 14, Case 2 and Case 5 have almost identical streamwise velocity profiles at the centerline. Both of these cases have the same pressure ratio of 1.25 and the flow is in low Kn transition regime. Cases 1, 4 and 6 all have the same pressure ratio of 2.50. The streamwise velocities at the centerline follow a similar trend expectedly. However, the magnitude of the streamwise velocities is different and the
difference increases throughout the channel with an increasing Kn number. Thus, despite having the same pressure ratio, Case 6 owns the fastest flow while the Case 1 has the slowest.

![Streamwise velocity distribution at the centerline](image)

Figure 16. Streamwise velocity distribution at the centerline

Case 6 has an inlet Knudsen number that is two times larger than that of Case 4 and twenty times larger than that of Case 1. However, the relationship between the rate of change of flow velocities is not linear with rate of increase in Kn numbers. Therefore, the effect rarefaction slows down after a certain Kn limit if the pressure ratio is kept the same.
Having the largest pressure ratio Case 3 has the fastest flow and largest slip velocities at the walls among all cases. It is interesting to see, the flow acceleration and slip at the upper wall during the one-sixth of the channel is very close to that of Case 6 with a lower pressure ratio. However, the velocity of Case 3 increases remarkably beyond one-third of the channel.

The distribution of local Kn through the channel is given in Figure 15. The decrease in the pressure is captured by the increase in Kn and similarly flow acceleration increases the velocity gradient at the wall. For the current problem insignificant changes are observed at different elevations in the channel. Therefore, for the sake of simplicity only the upper wall distribution is shown in the figure.

Figure 17. Distribution of Knudsen number in the streamwise direction.
The Kn numbers are calculated based on the flow height. Since the inlet section is narrow the corresponding Kn numbers are high in this region. The sudden drop occurs where the sudden enlargement is introduced.

The mean free path increases along the channel as the pressure drops. Due to introduction of the step feature, the slope of the pressure profile shows a steep change. Fluctuations occurring at the channel inlet vanish after the sudden enlargement. It is found that these result from the fluctuations happening in the sampled cell temperatures. A further investigation is needed to understand the reasons behind this oscillatory behavior.

Sharing the same exit pressures and exit temperatures, the exit Kn numbers for Cases 3, 4 and 5 are equal to each other. Similarly, Case 1 and Case 2 have the same exit Kn numbers as well.

The temperature profiles nearby the inlet section are shown in Figure 16. The profiles generally attain the parabolic shape. However, temperature jumps at the upper wall and on the step are different than each other. However, Case 5 is exceptionally smooth and symmetric. For all other cases, the temperature jump over the step is smaller than the jump on the upper wall.

Figure 17 shows flow temperature profiles at various downstream locations. Temperature difference between the upper wall and lower walls slowly recovers along the streamwise
direction. The symmetry at upper and lower walls is quickly realized for low Kn transition regime flows. As it can be seen from the figures, after the middle section of the channel, the temperatures at the upper and lower walls become symmetric for all cases.

![Inlet Temperature Profiles](image)

**Figure 18. Inlet Temperature Profiles**

Remarkably, the flow quickly becomes fully isothermal for the Case 2. The characteristic shape of temperature profiles is not visible for this particular case. A good agreement is obtained for Case 5 which has the same pressure ratio as Case 2. However, the lag in the upper-wall temperature at the inlet section is clearly visible for the Case 5 which has a ten times higher Kn.
By comparing Cases 1, 4 and 6, it is observed that the temperature jump at walls increases with increasing Kn numbers. In agreement with this statement, Case 3 has the largest temperature jump among all cases.

Figure 19 presents the pressure distribution along the streamwise direction for all of the cases. As expected, pressure decreases along the channel in a nonlinear fashion. This result agrees with the previous slip flow regime studies. A steep change in the slope of the pressure curve occurs where there is a sudden, unsymmetrical change in the flow area due to the step feature at the bottom wall.

Small fluctuations occur at the channel inlet. However, after the sudden enlargement, these fluctuations disappear. A quick investigation shows that these fluctuations result from the fluctuations in the sampled cell temperatures. A further investigation is needed to understand the reasons behind the phenomenon as the density distribution is smooth.
Figure 19. Temperature profiles at different streamwise locations. a) Case 1, b) Case 2, c) Case 3
Figure 20. Temperature profiles at different streamwise locations. a) Case 4, b) Case 5, c) Case 6
Figure 21. Pressure distribution along the channel for Case #1

The pressure distributions for different cases are shown in Figure 20. Expectedly, the distributions are nearly the same for the cases having the same pressure ratios.

Figure 22. Comparison of Pressure distributions
The comparison between case 1 and case 4 in Figure 21 demonstrates that as the Kn increases the pressure distribution becomes linear. This result agrees with previous findings of various authors.

![Lower Wall Pressures Case #1 (Kn=0.17) and Case #4 (Kn=1.7)](image)

**Figure 23. Pressure distribution comparison for low and high Kn cases**

On the other hand, as Kn goes from 0.347 to 3.47 in cases 2 and 6 respectively, the pressure distribution does not show a noticeable change. This might be due to the relatively low pressures and pressure ratios involved. However, it is evident that the flow properties become invariant due to rarefaction beyond a certain Kn limit. Future investigations are required to understand when exactly this phenomenon occurs.

The velocity fields are presented in Figure 22 and 23. The streamwise velocities are given without being normalized as can be encountered in many low-speed DSMC studies.
Inlet 0.25*L 0.50*L 0.75*L Outlet

Figure 24. Velocity fields at various streamwise locations a) Case 1, b) Case 2, c) Case 3.
Figure 25. Velocity fields at various streamwise locations a) Case 4, b) Case 5, c) Case 6
The next three figures show the streamwise velocity along the channel at different elevations in the channel.

Figure 26. Velocity distribution along the channel at various elevations a) case 1 b) case 2
Figure 27. Velocity distribution along the channel at various elevations a) case 3 b) case 4
Figure 28. Velocity distribution along the channel at various elevations a) case 5 b) case 6

The following figures present temperature distributions along the channel. Flow temperature and temperature jump at the walls are high at large Kn numbers.
Figure 29. Temperature distributions along the channel for a) case 1 b) case 2
Figure 30. Temperature distributions along the channel for a) case 3 b) case 4
Figure 31. Temperature distributions along the channel for a) case 5 b) case 6

For the second and fourth cases, the flow temperature reaches to a maximum and stays the same along the channel. However, temperatures drop slightly as the flow moves down the channel especially nearby the exit plane for all other cases.
The pressure ratio for the case 2 and 4 is equal to each other and the value, 1.25 is the lowest amongst all other cases. The temperature drop might be caused by cooling expansion of the gas at lower pressures which surpasses the viscous heating. The nonlinear change in temperature is more pronounced in the case number three which has the highest pressure ratio.

The case number six has the highest Kn having the lowest pressures at the channel ends. As it can be seen from the Figure 29, the flow temperatures experience a lag. Rather than a rapid, linear increase as in the rest of the cases, the temperature at the centerline of the inlet section (0.75H) follows a curvy pattern. Similarly, as the Knudsen number increases, the flow temperature reaches the maximum at a farther downstream location.

The heat flux distributions at the upper walls are shown in Figure 30. It is observed that the magnitude of the heat flux at the upper wall increases with increasing pressure and pressure ratio. Thus, it can be stated that the heat flux is inversely proportional to the Kn for subsonic flows.
The heat flux values at the bottom plates is nonzero although they are negligible compared to those of upper walls. However, for Boltzmann based particle approaches, it is normal to predict the wall heat transfer nonzero as the heat transfer is calculated from the net kinetic and rotational energy exchange of the particles striking to the wall.

Even with isothermal Couette flow geometry (Marques, 2000) in slip regime, while the Navier-Stokes and Fourier solution reads the heat flux parallel to the plates as zero, the non-linear term in the Burnett equation the heat flux does not become zero.

From the macroscopic point of view, the heat flux is proportional to the temperature gradient at the wall. This statement does not conflict with the temperature profiles.
obtained in the simulation. Additionally, considering the definition of the pressure, the number of collisions between the particles and the wall can be a factor for having relatively large heat fluxes where the pressure is high.

The next figure, Figure 31, is a magnified view of the lower wall heat flux for the first case. As it can be seen, the heat flux reaches a peak and then decreases to a value which will remain the same along the streamwise direction. It is noted that the fluctuations increase towards the channel end. Since the velocity and temperature boundary conditions are adjusted at every time step for the incoming molecules, the fluctuations do not disappear completely even for larger sampling sizes.

Figure 33. The magnified view of Lower-wall Heat Flux for the first case
On the other hand, the first case has the lowest Kn number amongst all of the cases. As mentioned earlier, the slight temperature drop is observed nearby the exit plane for cases with high Kn or high pressure ratios. Hence, the heat flux on the walls nearby the exit shows a unique behavior. This can be seen on the lower-wall heat flux better as the lower wall heat flux is small compared to upper wall heat flux. For brevity, the lower wall heat flux distribution is shown for the third case in the next figure.

![Figure 34. The magnified view of Lower-wall Heat Flux for the third case](image)

Although it is not possible to give a complete physical explanation, the same-type temperature drops nearby the exit plane are also observed by various authors who used the classical DSMC with the pressure boundary conditions. Therefore the drop might be related to incomplete equilibrium assumptions at the outlet boundaries when applying the
pressure boundary conditions. The extraction of the bulk flow energy from the thermal energies of the molecules might be another reason. However, more detailed numerical and experimental studies must be done to investigate and clarify the exact reasons behind this unique behavior.

It might be also critical to check mass and energy balance in the simulation. However, the IP method automatically updates the density values at each time step using the conservative form of the continuity equation. Therefore, the mass balance is automatically assured. Expectedly, mass flux calculations in different planes of the channels show that the errors of the mass flow rates are all within 2% in this study. For the sake of completeness, a sample mass flow rate distribution is shown for the third case.

Figure 35. The percent error of the mass flow rate for the third case
CHAPTER SIX: CONCLUSION

Gaseous backward facing step flow in a microchannel is simulated using the Information Preservation method based on Direct Simulation Monte Carlo. The numerical procedure and critical parameters are discussed.

The unidirectional IP method with periodic boundary conditions has been transformed into a two dimensions with a domain confined by two diffusive solid boundaries. The DSMC based code is further developed by implementing implicit inlet and outlet pressure boundary conditions. Inlet and outlet boundary conditions are varied to investigate flow behavior.

The success and future applications of DSMC only depend on the available computational resources. Although IP method is theoretically not explored well, it is a promising contribution that successfully reduces the unbearable statistical scatter of DSMC in low speed rarefied flows. Thus the IP method also facilitates application of proper boundary conditions for the DSMC and broadens the applicability of DSMC method in complicated and practical flow problems.

The computational cost increases due to IP as more variables and arrays are stored and several additional calculations are required. However, this additional cost is insignificant compared to the cost to reach impossible sampling sizes required by the standard DSMC
in low speed flows. The existence of recent studies involving impractical hypersonic microchannel flows is a clear indication of the necessity of IP-like methods in the field.

Future works may introduce modifications of the IP energy transfer procedure and improvements in determining molecular speeds at the domain-boundary cells. Additionally, when large time steps and less number of molecules are used in the simulation, sudden code interruptions occur due to empty computational cells and large statistical scatter especially at the beginning stages of the simulation. Although automatic time-step correction algorithm help, further precautions should be taken to prevent unexpected cut-offs.
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