Shock Tube Flow Simulations Using Direct Simulation Monte Carlo Method

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Abstract. *The Direct Simulation Monte-Carlo method (DSMC) is the standard computational method for rarefied flows, where the governing equation is the Boltzmann equation. In DSMC, the flow is represented by a large number of simulator particles and the evolution of the flow is tracked by calculating the motion of these particles and their collisions amongst themselves and with any boundaries of the domain. Due to an increased interest at CTA on reentry and/or rarefied flow conditions, the available simulation capabilities of the Computational Aerodynamics Laboratory are being extended to also include very low density flows. The paper presents results of the use of the DSMC method for shock tube flows and for the flow over a flat plate obstacle positioned perpendicular to the freestream. The results obtained so far indicate that the capability presently implemented seems to follow the expected tendency of recovering the usual Navier-Stokes continuum behavior as the Knudsen number is reduced. The results demonstrate the current status of the development of the desired capability and they contribute to the validation process of such implementation.*

Keywords: *Rarefied Flows, DSMC, Aerospace Applications, Shock Tube Flows*

1. INTRODUCTION

The Navier-Stokes equations commonly encountered in fluid mechanics applications are built upon the continuum approximation. When the ratio of the mean free path λ to the macroscopic length scale L, formalized by the non-dimensional Knudsen number, $Kn = \lambda/L$, becomes large, this approximation breaks down. The macroscopic length scale should be based on the local field, *i.e.*, velocity, pressure, density, to gradient ratio, thereby removing the question on how to define this length scale for complex flows. For small Knudsen numbers $Kn < 0.1$, the continuum approximation is valid. However for larger Knudsen numbers, one has to resort to some methodology which considers interaction between particles. The Boltzmann equation is the accepted mathematical model of a gas flow at the molecular level. Numerically, this equation can be solved using conventional CFD techniques, with the velocity distribution function being the solution obtained in a computational grid. Since this is a 6-dimensional partial differential equation, it quickly becomes computationally heavy. Further, the evaluation of the collision terms in the Boltzmann equation, represented by the right hand side integrals, is a challenging task.

An alternative to the solution the Boltzmann equation is to employ direct simulation methods, where a large number of simulated molecules are tracked in space and time, and their velocities and internal states are modified through collisions and boundary interactions. One of such approaches is the Direct Simulation Monte Carlo (DSMC) method, is the standard computational method for rarefied flows. In DSMC, as discussed, the flow is represented by a large number of simulator particles and the evolution of the flow is tracked by calculating the motion of these particles and their collisions amongst themselves and with any boundaries of the domain. The simulation is advanced in time steps of duration Δt which, for accuracy, should be less than the mean time between collisions. During each time step the convection and collision calculations are decoupled. First, the particles are moved in collisionless flight, according to their velocities. Next, the particles are frozen in position and binary collisions are calculated for some of the particles. Post-collision velocities are calculated for the given relative speed of collision and a randomly chosen set of impact parameters. The probability of collision for each collision pair, and the total number of collisions, reflect the theoretical correct probability and total collision rate for the particular collision cross-section used. In the next section, some aspects of the probabilistic approach to direct simulation methods are briefly described.

2. DESCRIPTION OF THE DIRECT SIMULATION METHOD

The Direct Simulation Monte Carlo (DSMC) (Bird, 1994) method is suitable for simulating the behavior of dilute gases by means of a probabilistic approach. The term dilute gas means that a typical molecular spacing δ is much larger than a typical molecule diameter d, formally stated as $\delta/d > 1$. In terms of Knudsen number (Kn), this would approximately mean that $O(0.1) \leq Kn \leq O(10)$. The fundamental idea of DSMC is to track a large number of statistically representative particles, where each of the particles contains a cluster of molecules. The particle motion and interactions are used to modify their positions and velocities. The DSMC procedure consists of four main stages, namely: move the particles, keep track of the position, perform collisions using probabilistic methods and sample the flow field.

2.1 Cell and Sub-cell Width

Although particles are allowed to cross the borders of the cells, individual collisions occur with neighbors in the same cell. More specifically, the DSMC method uses the sub-cell approach, where local collision rates are based on the individual cells, but the possible collision pairs are restricted to sub-cells. A rule of thumb is that the cell width should be $\Delta x = \lambda/3$, where λ is the mean free path. This quantity can be estimated from the formulation based on the hard sphere assumption (Bird, 1994).

$$\lambda = \frac{\overline{c'}/\bar{c}_r}{n\pi d^2} \approx \frac{1}{n\pi d^2} \,, \tag{1}$$

where n is the number density, δ the molecular diameter and $\overline{c'}$ is the mean thermodynamic velocity magnitude defined by Eq. (2),

$$\overline{c'} = \sqrt{2T_o\kappa/m} \,. \tag{2}$$

In the present formulation, T_o is the reference temperature, *i.e.*, $T_o = 273$, κ is the Boltzmann constant, and m is the molecular mass. Moreover, the reader should observe that $\bar{c}_r$ is the average relative velocity magnitude. The sub-cell width should be taken to be small in comparison to λ. Typically, this would mean $\Delta x_s \approx 0.1\Delta x$, where Δx_s is the sub-cell width.

2.2 Time Step

In the DSMC method, there is no stability limit connected to the choice of the time step, Δt. There is, however, from a physical point of view, a limitation given by the mean collision time, essentially stating that the time step should be sufficiently small in order to uncouple the molecular motions and collisions. An estimate to this time step can be given for a hard sphere as

$$\Delta t = \frac{\lambda\pi}{2\overline{c'}} \,. \tag{3}$$

2.3 Particles

Instead of simulating the action of every molecule, the DSMC method clusters a large set of molecules, subsequently tracking each of these clusters as individual "particles" in time and space. The number of molecules contained in each particle should be adequately chosen in such a manner that statistical fluctuations do not become too large. A reasonable amount of molecules contained in each particle (F_N) is $10^{14} < F_N < 10^{18}$. Therefore, it necessary to compute the evolution of between 10^2 and 10^6 particles for a number density of $n = 10^{20}$.

2.3.1 Moving Particles

At every time step, the particles are moved to their new position according to

$$\vec{r}(r + \Delta t) = \vec{r}(t) + \vec{v'}(t)\Delta t \,, \tag{4}$$

assuming that no interactions have occurred during this time interval. After the particles are moved, boundary conditions are enforced.

2.3.2 Indexing

After having moved all the particles according to their velocities, a reindexing is performed. This implies that, in all sub-cells, the number of particles are counted and, then, each particle is given a specific address.

2.4 Boundary Conditions

The boundary conditions implemented in the present work consider solid surface specular reflection. Specular reflection reverses the velocity component normal to the surface, while those components parallel to the surface are unchanged. The final position of the molecule that strikes a surface normal to the x-axis at x_c, and would have moved to $x^{'}$ beyond it, is given by

$$x_c - x = x^{'} - x_c \,, \tag{5}$$

or

$$x = 2x_c - x^{'} \,. \tag{6}$$

2.5 Collisions

In the DSMC procedure, only particles within a cell are paired up in order to perform collisions. Since we are dealing with dilute gases, there is an overwhelming probability that the collisions will be binary,*i.e.*, involving only two particles. If one considers a time interval Δt, in a DSMC cell of volume V_c, containing N simulated particles, each representing F_N number of molecules, then the number of collisions that might occur is easily recognized to be $N(N-1)/2$. This yields that the probability for each of the collisions becomes

$$P = F_N \sigma_T c_r \Delta t / V_c \,, \tag{7}$$

where σ_T is the total collision cross section and c_r is the relative velocity of the pair of particles considered as we can observe in Figs. 1 and 2. A straightforward method is to look for possible collision pairs by considering all $N(N-1)/2$

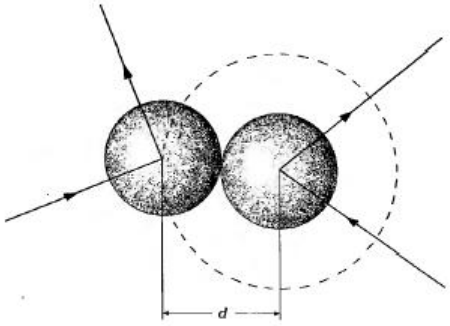

Figure 1. Collision cross section σ_T between two hard spheres of diameter d.

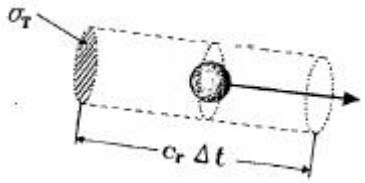

Figure 2. Effective volume swept out by moving molecule.

potential collisions using a random selection procedure, together with the probability P. However, due to the large number of particles, N, and the low probability, P, this procedure is computationally challenging, requiring a computational time proportional to N^2. In order to make the computational time linear with N, the DSMC approach uses the so-called NTC (no time counter) method in which a normalized probability is introduced. Hence, one can write that the maximum collision probability is

$$P_{max} = \frac{FN(\sigma_T c_r)_{max} \Delta t}{V_c} \,, \tag{8}$$

where $(\sigma_T c_r)_{max}$ is a precomputed maximum collision cross section of the cell. Based on this approach a number of representative collisions is computed as

$$1/2 N \overline{N} F N (\sigma_T c_r)_{max} \Delta t / Vc \,. \tag{9}$$

Here, $\overline{N}$ is a time ensembled average of particles contained in the cell. For each of these possible collisions, the procedure now picks a random particle and finds its corresponding sub-cell. Within this sub-cell, it picks another random particle so that these two form a collision pair. The collision is now computed with the probability

$$P = \frac{\sigma_T c_r}{(\sigma_T c_r)_{max}} \,. \tag{10}$$

This essentially means that a random number is compared to the above fraction and, if it is bigger, we have a collision. Otherwise, it is assumed that there is no collisions. The collisions themselves are modelled as different variants of a hard sphere collision. In the hard sphere approximation, elastic collisions are assumed, yielding a conserved magnitude of the relative velocities of the two particles. It, hence, becomes necessary only to compute the direction of the particles after the collision, also known as the angle of deflection χ. The angles are computed with random samples for the hard sphere case, but alternative implementations are those of a variable hard sphere (VHS) and a variable soft sphere (VSS) (Bird,1994).

3. RESULTS

3.1 Zero-dimensional Gas

As a simple simulation, the DSMC procedure was tested in a homogeneous, or "zero-dimensional" gas. In the language of Bird (1994), a "zero-dimensional," gas is a gas with no macroscopic gradients. Likewise, a "one-dimensional" gas is a gas with macroscopic gradients in only one direction. Although the gas is homogeneous, a one-dimensional computational domain $x \in [0, 1]$ is considered. The boundary conditions are specular reflections at both boundaries. The present test case has an initial equilibrium where the velocity distribution is given by the Maxwell-Boltzmann distribution (Pullin, 1980). The material properties of the gas are the flollowing: the molecular mass is $m = 5 \times 10^{-26}$, the molecular diameter is $d = 3.5 \times 10^{-10}$ and the number density is $n = 10^{20}$. The number of cells is $M_c = 50$ and each cell has 8 sub-cells. The time step is taken to be $\Delta t = 2.5 \times 10^{-5}$. The computational cost of the procedure is mainly determined by the ratio of the number density, n, to the number of molecules F_N simulated by each particle, since the number of simulated particles is $N = n/F_N$. If F_N is too large, the simulation is subject to statistical fluctuations and, conversely, if F_N is too small, the computational effort will be extremely high. One can observe in Fig. 3 the number density as a function of x (cell centroid values) starting with initial equilibrium. Statistically, in each cell, the number density should be 10^{20}. From the dashed line in this plot, it can be seen that, when choosing $F_N = 10^{19}$, implying that only 10 particles are simulated, the statistical fluctuation is very large. As one decreases F_N, the fluctuations also decrease, and a resonable value of F_N in the present application seems to be $F_N = 10^{15}$, as presented by the solid line without any symbols in Fig. 3. Table 1 presents the normalized standard deviation of the number density for the cases shown in Fig. 3. The Knudsen number used for the present test case is $K_n = 1.0$, and the final time considered is $t = 3.0$ s (physical time), for all simulations.

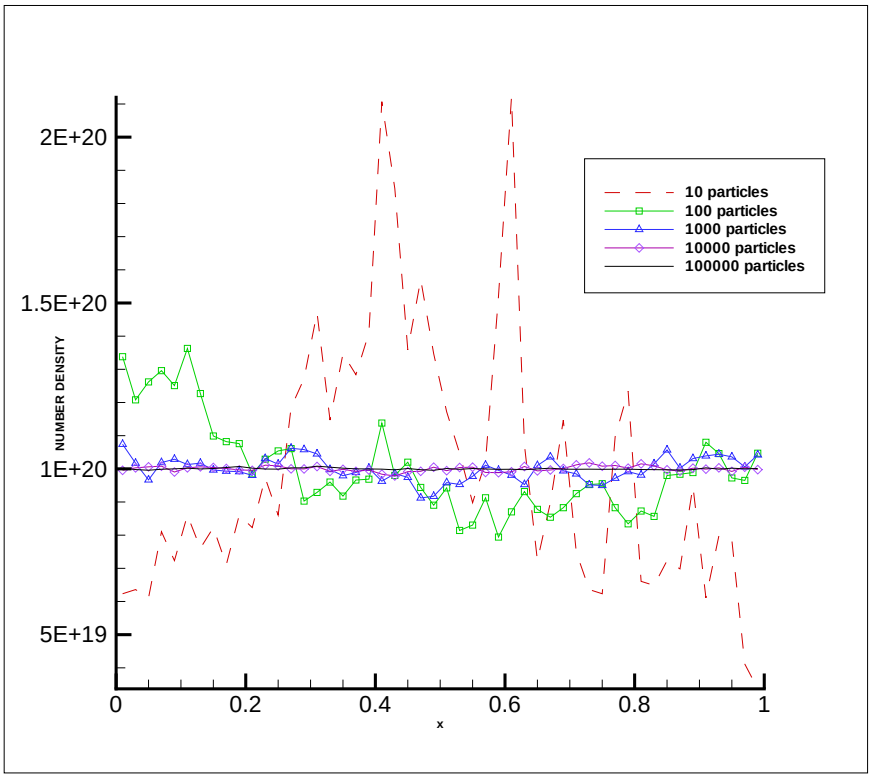

Figure 3. Number density for different number of simulated molecules per particle, F_N.

3.2 One-dimensional Shock-tube Problem

As previously defined, a "one-dimensional" gas is a gas with macroscopic gradients in only one direction. The same one-dimensional computational domain, with $x \in [0, 1]$, is considered. The boundary conditions are specular reflections at both boundaries. In order to test the present numerical method and to show the effect of rarefaction in the shock-tube flow, the problem is set with initial states: $\rho = 10$, $U = 0.0$, for $0.0 \leq x \leq 0.5$, and $\rho = 1.0$ and $U = 0.0$, for $0.5 < x \leq 1.0$. The material properties of the gas are the flollowing: molecular mass is $m = 5 \times 10^{-26}$, molecular diameter is $d = 3.5 \times 10^{-10}$. The number of cells is $M_c = 50$ and each cell has 8 sub-cells. The computed results in terms of density and pressure, for the cases of $K_n = 0.01$ and 0.1, at time $t = 0.15$ s, are shown and compared with the

Table 1. Normalized standard deviation of the number density as a function of the number of particles simulated.

Number of particles (N)	Normalized standard deviation (%)
10 particles	39.27
100 particles	13.84
1000 particles	3.58
10000 particles	0.81
100000 particles	0.26

analytical solutions obtained using the equations of gas dynamics for continuum flow.

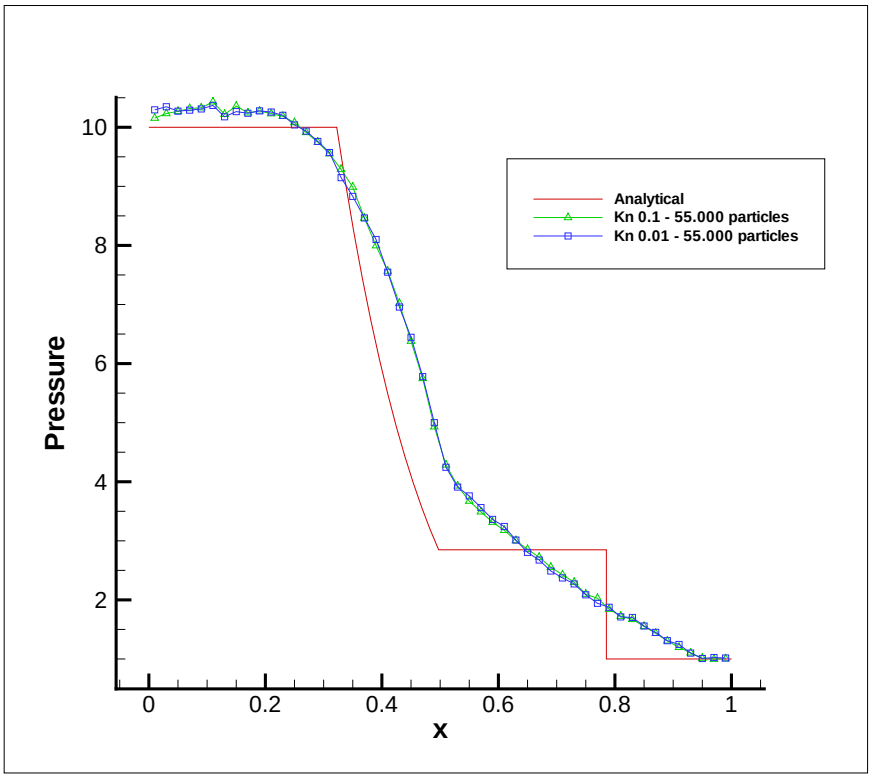

Figure 4. Dimensionless pressure for different Knudsen numbers.

The behavior to be expected is that, as the Knudsen number increases from $K_n = 0.01$ to $K_n = 0.1$, the shock wave should become thicker. One should further observe that, for a Knudsen number of about $K_n = 0.1$, the flow can already be considered as rarefied and, therefore, it is to be expected that the flow will still have strong gradients, but without a shock wave in the standard continuum sense. As the Knudsen number is decreased, the shock wave and the expansion fan profiles should become crisper. The results in Fig. 4 have not yet achieved the very crisp profiles, but they are showing the correct trend as one decreases the Knudsen number. A close observation of the DSMC result curves in the figure indicates that the calculations for $K_n = 0.01$ are slightly closer to the theoretical continuum result. It is clear, however, that there is room for improvement in the results. On the other hand, if one compares the curve for $K_n = 0.1$, in Fig. 4, with similar results in Li and Zhang (2004), it also becomes clear that the present calculations for the higher value of the Knudsen number are actually quite good (see Fig. 3 in Li and Zhang, 2004). Therefore, the conclusion is that a larger number of particles is necessary to simulate the flow at $K_n = 0.01$. In other words, since both simulations, at $K_n = 0.01$ and at $K_n = 0.1$, were performed with 55,000 particles, there are not enough particles for the lower Knudsen number case, although the solution is already quite good for the higher Knudsen number test case. The authors are currently running two similar shock tube simulations at $K_n = 0.01$, but using 550,000 and 5,500,000 particles, respectively, in each of these test cases. Unfortunately, due to the very large computational times, the results are not yet available at this time.

The computed dimensionless density profile are shown in Fig. 5. In a similar fashion as in the previous discussion, the computed densities near the shock wave and the expansion fan deviate from the exact solution of the continuum inviscid gas dynamics. Such deviation should become more prominent with increasing Knudsen number, and the deviation should gradually vanish when the Knudsen number diminishes towards the continuum flow regime. However, when decreasing

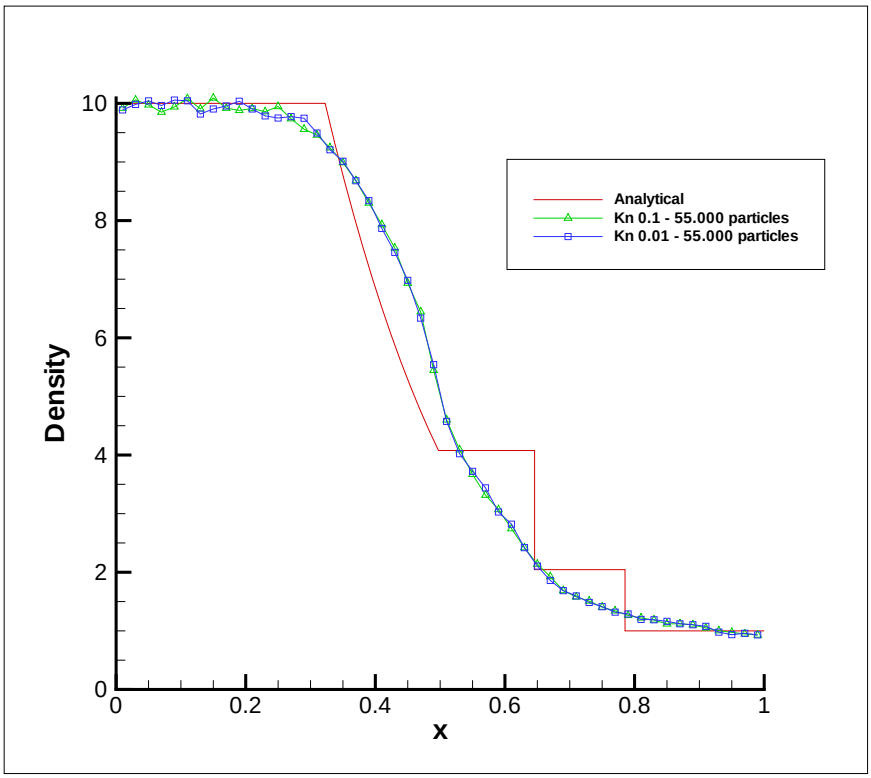

Figure 5. Dimensionless density for different Knudsen numbers.

the Knudsen number, it would be necessary to increase the number of particles used in the simulation in order to obtain the necessary support to correctly capture the shock wave and expansion fan, as already discussed. It should be further emphasized that all numerical results here discussed have been obtained for rarefied flows. The analytical results presented for comparison in this test case consider a continuous flow condition. Hence, one should not really expect that the rarefied flow simulations would have a perfect match with the analytical, continuous data.

3.3 Two-dimensional Flat Plate

A 2-D flat plate configuration, positioned perpendicularly to the flow, is also considered as a test cas in the present work. Although the extension of the simulation capability to the two-dimensional case is still ongoing, the preliminary results for the present test case are very interesting. The flow simulation problem is set with initial states: $U = 1400$ m/s and $V = 0$. The material properties of the gas are the following: the molecular mass is $m = 5 \times 10^{-26}$, the molecular diameter is $d = 3.5 \times 10^{-10}$. The time step is $\Delta t = 4.0 \times 10^{-6}$ and the total number of iterations is taken to be 10^6. The grid used in the simulation is made up of 600 cells, as one can observe in Fig. 6. The flat plate obstacle is positioned at $x = 0.5$, and in the range $y \in [0.25, 0.35]$. In other words, the plate is positioned exactly in the center of the computational domain indicated in Fig. 6. The qualitative results, in terms of density and temperature contours, for the case of $K_n = 0.1$, are shown in Figs. 7 and 8, respectively. The density and temperature contours indicate that the overall flow features are correctly captured by the present simulation. Hence, one can clearly see the formation of the detached bow shock wave in front of the blunt obstacle, as well as the heating at the face of the obstacle and the flow expansion as it moves downstream around the plate edges. Clearly, further validation of such simulations is still necessary, and this effort will be performed as the development of the 2-D simulation capability progresses.

4. CONCLUDING REMARKS

The direct simulation Monte Carlo (DSMC) method based on the molecular movement and collisions has been presented. It has been shown in the calculations here reported that the results of the present method are sensitive to the number of particles used in the simulations. The larger the number of particles used to represent the real molecules in the computation, the better should be the quality of the results. Clearly, however, this occurs at the expense of large computational memory and time usages. In the DSMC method, there are statistical fluctuations that require the number of particles to be sufficiently high. In general, for rarefied flow problems, the computational efficiency of the present method seems better than that of a Navier-Stokes solver. However, in the computation of a continuum flow, as the molecular mean

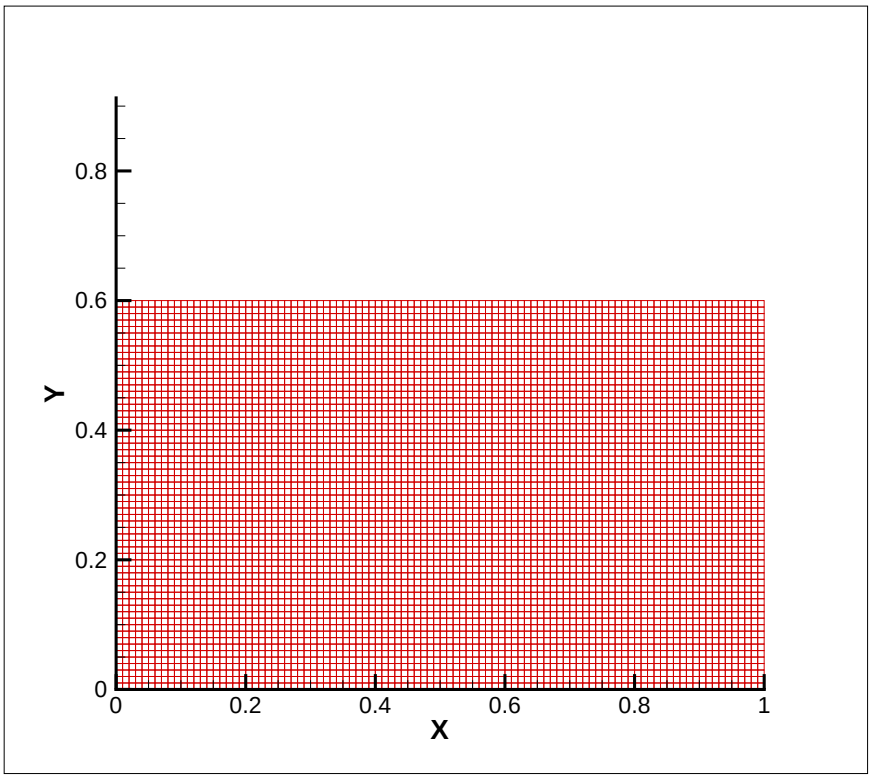

Figure 6. 2-D cartesian grid used in the simulation.

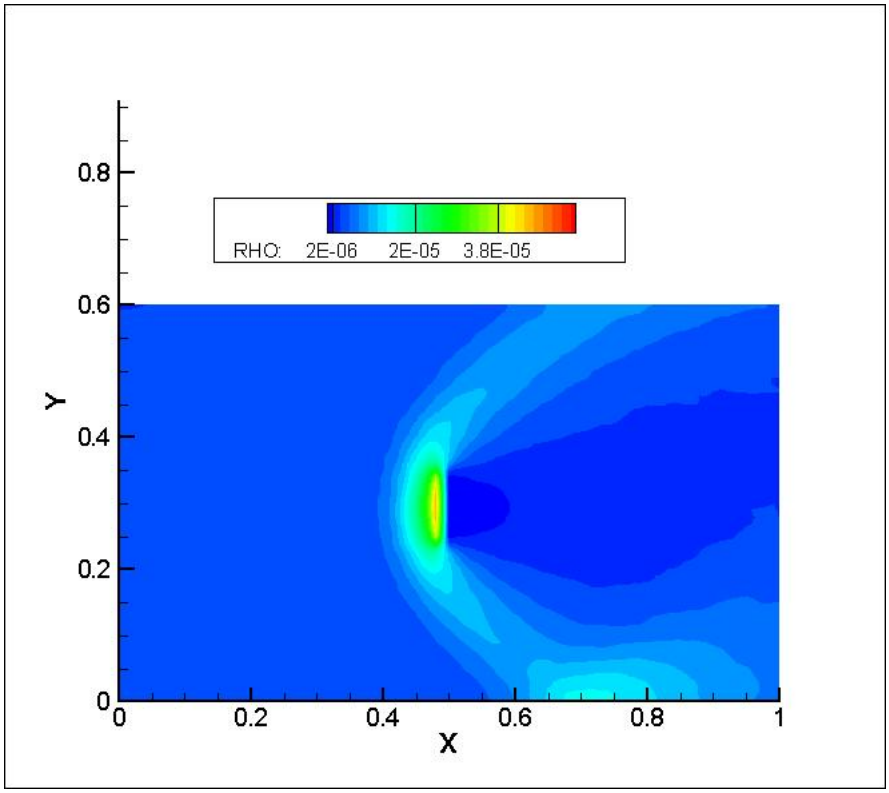

Figure 7. Density contours in the flat plate configuration.

collision time is generally smaller than the time step determined by the stability condition of the discrete schemes, the computational time step given by Eq. (3) will be quite small, sometimes even at a magnitude of 10^{-5}. As a result, the convergence rate of the present method will be slower than that of the Navier-Stokes solver for the continuum flow regime.

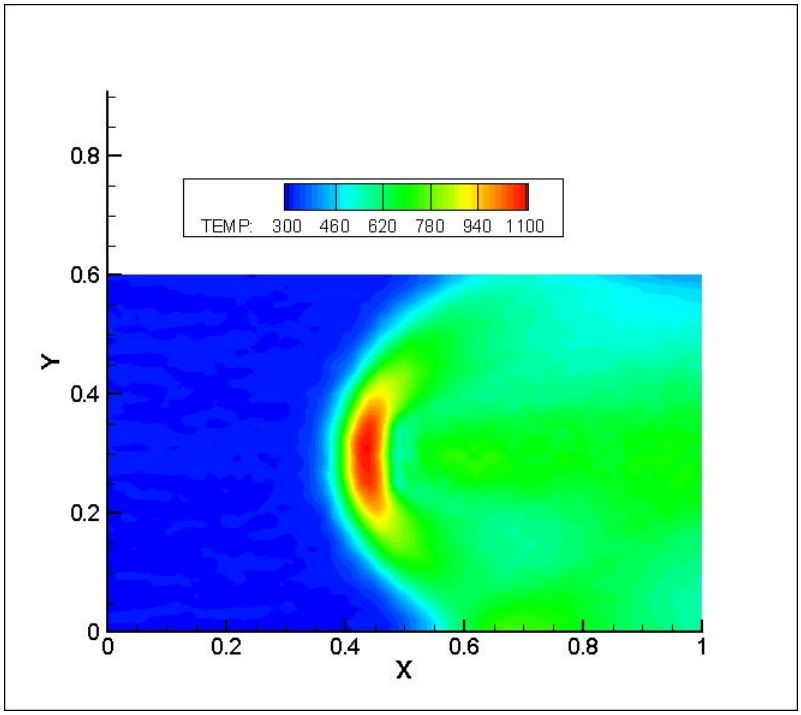

Figure 8. Temperature contours in the flat plate configuration.

It has been shown by the present computations that the computational time required by the DSMC method increases as the Knudsen number decreases.

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6. REFERENCES

Bird, G.A., 1970, "Breakdown of Translational and Rotational Equilibrium in Gaseous Expansions," AIAA Journal, Vol. 8, No. 11, pp. 1998-2003.

Bird, G.A., 1994, "Molecular Gas Dynamics and the Direct Simulation of Gas Flows," Oxford University Press Inc., New York.

Larsen, P.S., and Borgnakke, C., 1975, "Statistical Collision Model for Monte Carlo Simulation of Polyatomic Gas Mixture," Journal of Computational Physics, Vol. 18, pp. 405–420.

Li, Z. and Zhang, H., 2004, "Study on gas Kinetic Unified Algorithm for Flows from Rarefied Transition to Continuum," Journal of Computational Physics, Vol. 193, pp. 708–738.

Moreira, F.C., 2007, "On The Behavior of Upwind Schemes Applied to Three-Dimensional Supersonic and Hypersonic Cold Gas Flow Simulations of Aerospace Configurations," Master Thesis, Instituto Tecnológico de Aeronáutica, São José dos Campos, SP, Brazil.

Morinishi, K., 2006, "Numerical Simulation for Gas Microflows using Boltzmann Equation," Journal of Computational Physics, Vol. 35, pp. 978–985.

Moss, J.N., Dogra, D. B., Price, J. M., and Hash, D.B., 1995, "Comparison of DSMC and Experimental Results for Hypersonic External Flow," AIAA Paper No. 95–2028.

Pullin, D.I., 1980, "Direct Simulation Methods for Compressible Inviscid Ideal-Gas Flow," Journal of Computational Physics, Vol. 34, pp. 231–244.

Wright, M.J., D. K.P. and Martinez, E.R., 2006, "Analysis of Apollo Comand Module Afterbody Heating Part I: AS-202," Journal of Thermophysics and Heat Transfer, Vol. 20, pp. 16–30.