DIRECT SIMULATION MONTE CARLO METHOD IN HYPERSONIC RAREFIED GAS FLOW SIMULATIONS IN FLAT PLAT GEOMETRY

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Abstract. *Direct Simulation Monte-Carlo method (DSMC) is the standard computational method for rarefied flows, which can be more appropriately represented by 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 the flow over a flat plate obstacle positioned parallel to the freestream. The results obtained so far demonstrate the current status of the development of the desired capability and they contribute to the validation process of such implementation.*

Keywords: *DSMC, Rarefied Flows, Hypersonic*

1. INTRODUCTION

The Direct Simulation Monte Carlo method (Bird, 1970) is the most useful numerical method for solving problems where the flow is considered rarefied. The dimensionless parameter used to describing the degree of gas rarefaction is denoted by the Knudsen number

$$K_n = \frac{\lambda}{L} \tag{1}$$

i.e. the ratio of the mean free path λ to the macroscopic length scale L. 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. The Navier-Stokes equations commonly encountered in fluid mechanics applications are built upon the continuum approximation. For small Knudsen numbers ($Kn \sim 0.01$), the continuum approximation is valid. However for larger Knudsen numbers, this approximation breaks down and one has to resort to some methodology which considers interaction between particles (Li and Zhang, 2004). 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 (Moreira, 2007) 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 (Morinishi, 2006), 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. The basis of the DSMC method, first formulated by Bird (1970), is to circumvent the direct solution of the Boltzmann equation by considering a probabilistic simulation. It is categorized as a particle method, in which each simulation particle represents a large number of real gas atoms or molecules. The physics of the gas is captured by uncoupling the motion of the particles from their collisions. In a similar manner to conventional CFD, the implementation of DSMC normally requires the decomposition of the computational domain into a collection of grid cells. After molecular movements have taken place, the collisions between particles are simulated in each cell in a probabilistic manner and a statistical picture of the flow phenomena is built up. 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 (Wright *et al.*, 2006). 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.

With the advent of high performance computing architectures, practical solutions to engineering problems in smaller 2D geometries may be achieved nowadays within realistic time scales using a modest PC. The DSMC code presented in this paper is based on Bird's formulation (Bird, 1994).

2. NUMERICAL PROCEDURES

The Direct Simulation Monte Carlo (DSMC) (Pullin, 1980) 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. Basically, 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

In a similar manner to conventional CFD, a numerical mesh is created to describe the physical extent of the flow domain and any solid obstacles within it. Good DSMC practice suggests that the typical cell size should be a fraction of the mean free path. A rule of thumb is that the cell width should be determined by the following equation:

$$\Delta_x = \frac{\lambda}{3}\,, \tag{2}$$

where Δ_x is the cell width and λ is the mean free path estimated from the formulation based on the general molecular model hard sphere (Bird, 1994).

$$\lambda = \frac{1}{\sqrt{2}\pi d^2 n}\,. \tag{3}$$

where d is molecular diameter and n is the number density. 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. 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. The 2-D Cartesian grid used by the numerical code is presented in Fig.1.

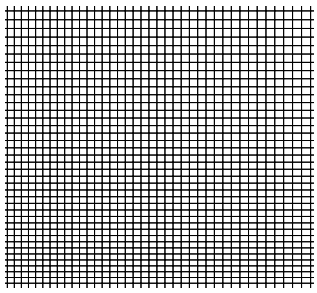

Figure 1. cartesian grid used in the simulations

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 a fraction of the mean collision time of the gas molecules in order to uncouple the molecular motions and collisions. An estimate to this time step can be given as

$$\Delta t = \frac{\lambda\pi}{2\overline{c'}}\,, \tag{4}$$

where $c^{'}$ is the mean thermodynamic velocity magnitude defined by

$$\overline{c'} = \sqrt{2T_o\kappa/m}\,. \tag{5}$$

In the present formulation, T_o is the reference temperature, *i.e.*, $T_o = 273$, κ is the Boltzmann constant, *i.e.* $\kappa = 1.380622 \times 10^{-23}$, and m is the molecular mass, *i.e.* $m = 4.65 \times 10^{-26}$.

2.3 Particles movement

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 as published by (Moss *et al.*, 1995). A reasonable amount of molecules contained in each particle (F_N) is $10^{14} < F_N < 10^{18}$. At every time step, the particles are moved to their new position according to

$$\vec{r}(r + \Delta t) = \vec{r}(t) + \vec{v^{'}}(t)\Delta t \,, \tag{6}$$

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

$$x_c - x = x^{'} - x_c \,, \tag{7}$$

or

$$x = 2x_c - x^{'} \,. \tag{8}$$

2.5 Collisions

In the DSMC procedure, only particles within a cell are paired up in order to perform collisions (Larsen and Borgnakke, 1975). 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

$$P = F_N \sigma_T c_r \Delta t / V_c \,, \tag{9}$$

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. 2 and 3. A straightforward method is to look for possible collision pairs by considering all $N(N-1)/2$

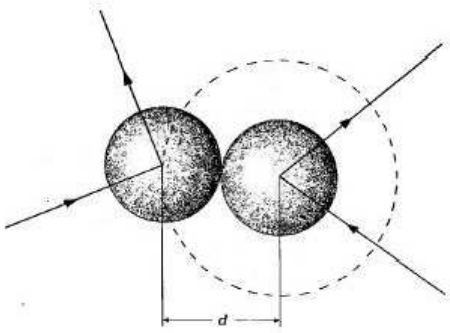

Figure 2. Collision cross section σ_T between two hard spheres of diameter d.

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

$$P_{max} = \frac{FN(\sigma_T c_r)_{max}\Delta t}{V_c} \,, \tag{10}$$

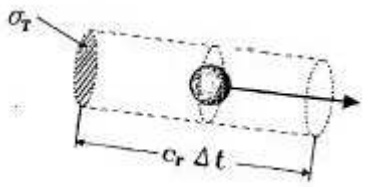

Figure 3. Effective volume swept out by moving molecule.

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

$$1/2N\overline{N}FN(\sigma_T c_r)_{max}\Delta t/Vc\,. \tag{11}$$

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

$$P = \frac{\sigma_T c_r}{(\sigma_T c_r)_{max}}\,. \tag{12}$$

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 AND DISCUSSION

A 2-D flat plate configuration, positioned parallel to the flow, is considered as a test case 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. Time averaging of the instantaneous DSMC particle fields was performed once steady-state had been achieved. The solution was considered to be steady when the average linear kinetic energy of the system showed only small changes with time. An example of this is shown in Fig. 4.

3.1 2-D supersonic flow over a flat plate at Mach 4.8

The flow simulation problem is set with initial states: $U = 1400$ m/s and $V = 0$ m/s. The material properties of the gas are the following: the molecular mass is $m = 5 \times 10^{-26}$ kg, the molecular diameter is $d = 3.5 \times 10^{-10}$ m. The time step is $\Delta t = 4.0 \times 10^{-6}$ s and the total number of iterations is taken to be 2^5. The grid used in the simulation is made up of 600 cells, as observed in Fig.1. The flat plate obstacle is positioned in the range $x \in [0.4, 0.6]$ m. The total number of DSMC particles in the system at steady-state was 36,000 and the cpu run-time was 4 h using a single AMD Turion Dual Core 64-bit, 2.2 GHz chip. Qualitative results, in terms of temperature and Mach number contours, for the case of $K_n = 0.01$, are shown in Figs. 5 and 6, respectively. The temperature and Mach number 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 flat plate obstacle. In Fig. 7 one can observe the temperature distribution over all the flat plate direction. The detached shock wave in front of the flat plate indicate a temperature increase before the flat plate from the far field temperature of 273 K up to 700 K in the beginning of the plate. The same effect can be observed in the scalar velocity distribution over the flat plate direction domain Fig. 8. The far field velocity is 1400 m/s, the detached shock wave improve decrease in the velocity profile before the plate and . As one can observe, good results are achieved for temperature and velocity profile.

3.2 2-D supersonic flow over a flat plate at Mach 2.4

The flow simulation problem is set with initial states: $U = 700$ m/s and $V = 0$ m/s. The material properties of the gas are the following: the molecular mass is $m = 5 \times 10^{-26}$ kg, the molecular diameter is $d = 3.5 \times 10^{-10}$ m. The time step is $\Delta t = 4.0 \times 10^{-6}$ s and the total number of iterations is taken to be 2^5. The grid used in the simulation is made up of 600 cells, as observed in Fig.1. The flat plate obstacle is positioned in the range $x \in [0.4, 0.6]$ m. The total number of

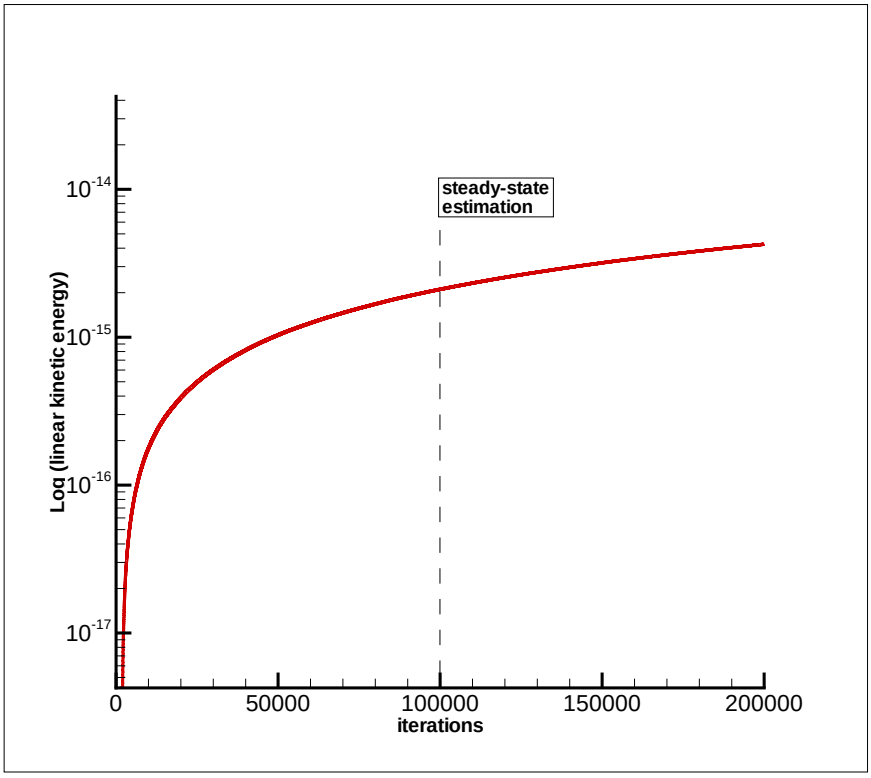

Figure 4. Estimation of steady-state conditions

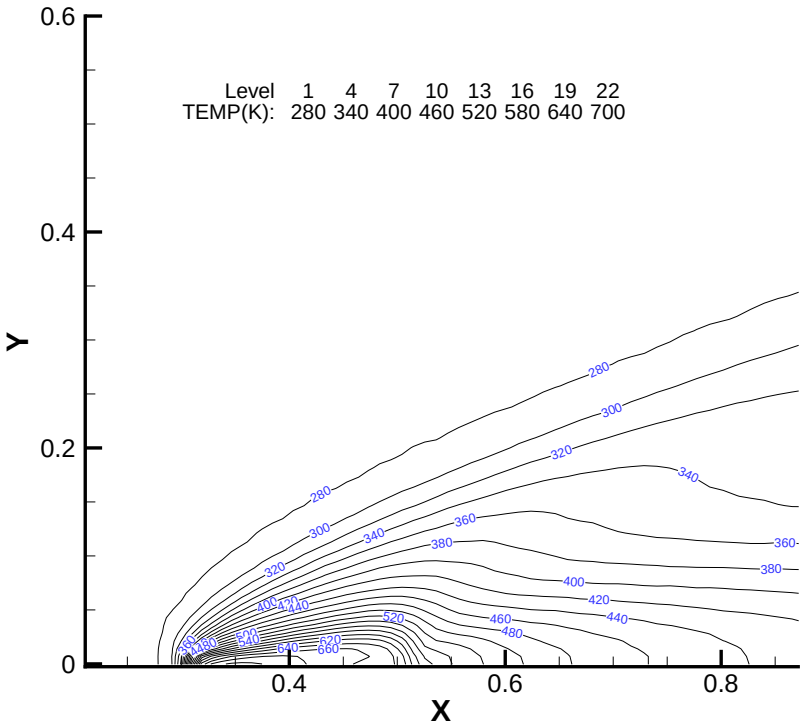

Figure 5. Temperature contours in the flat plate configuration for free stream Mach number 4.8.

DSMC particles in the system at steady-state was 36,000 and the cpu run-time was 4 h using a single AMD Turion Dual Core 64-bit, 2.2 GHz chip.

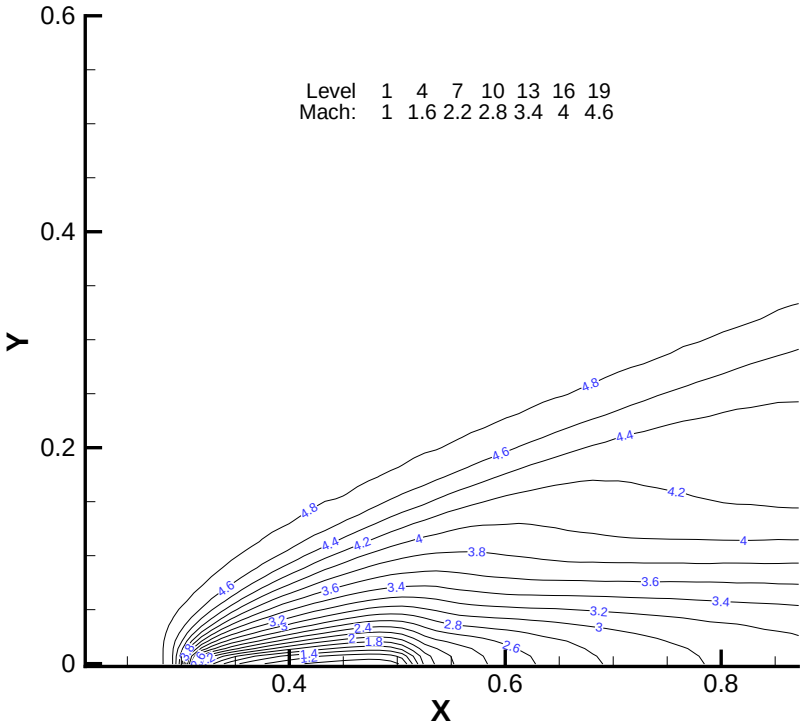

Figure 6. Mach number contours in the flat plate configuration for free stream Mach number 4.8.

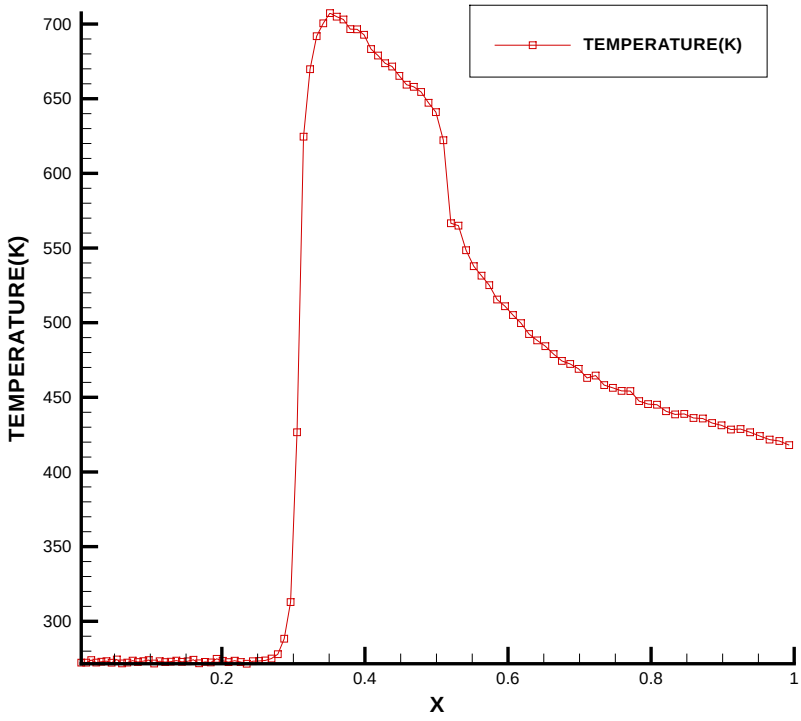

Figure 7. Temperature distribution profile throughout the flat plate configuration for free stream Mach number 4.8.

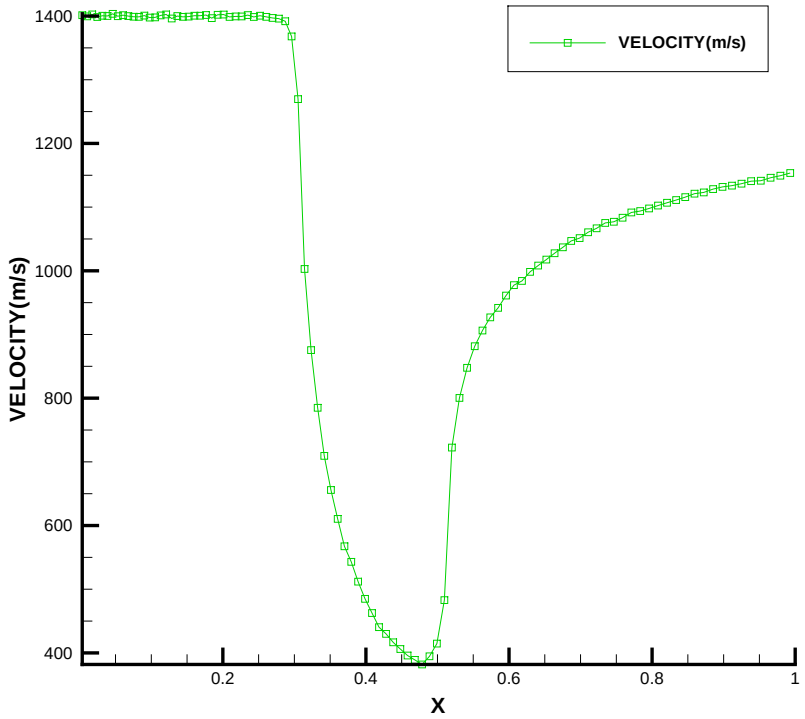

Figure 8. Velocity distribution profile throughout the flat plate configuration for free stream Mach number 4.8.

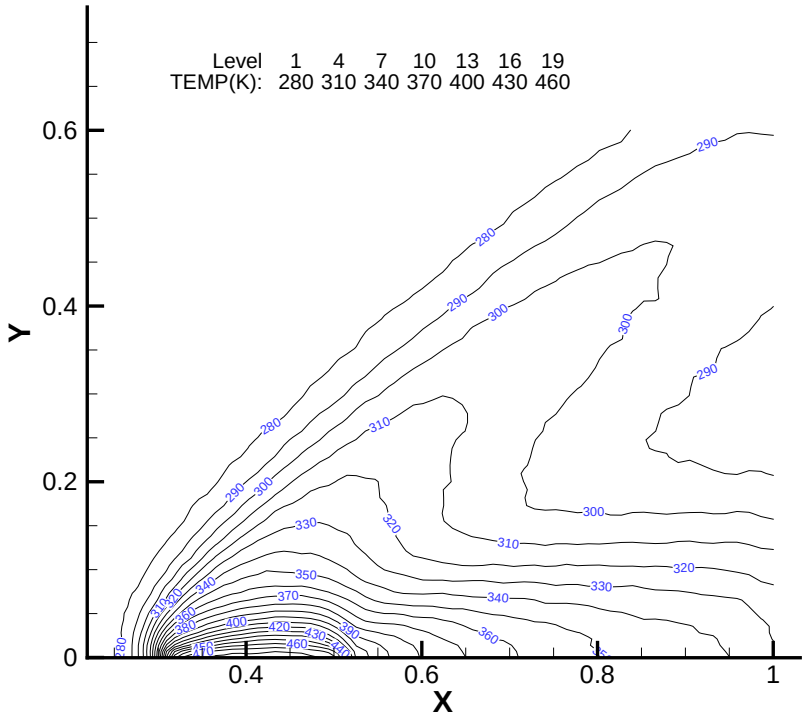

Figure 9. Temperature contours in the flat plate configuration for free stream Mach number 2.4.

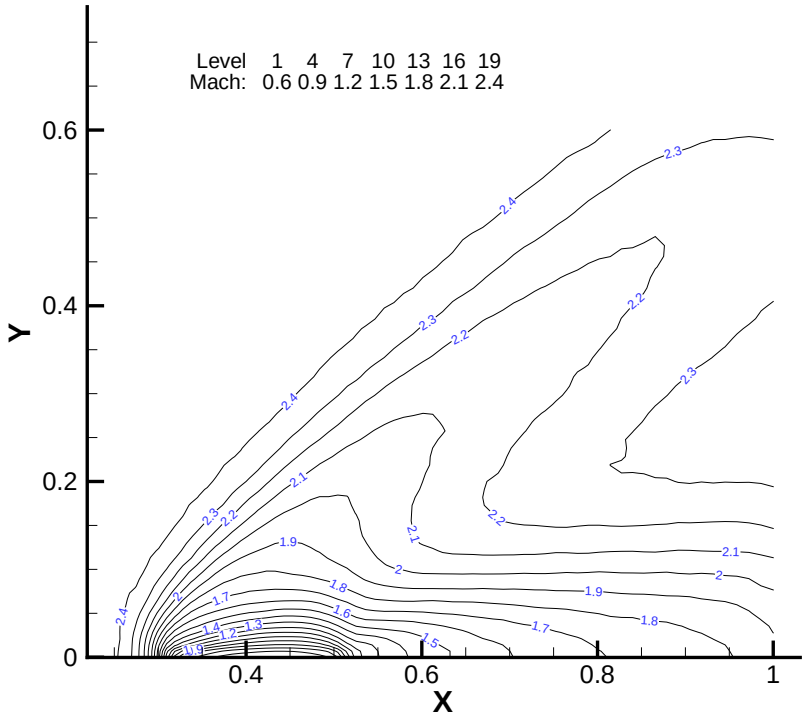

Figure 10. Mach number contours in the flat plate configuration for free stream Mach number 2.4.

The temperature and Mach number contours for free stream Mach number 2.4, also indicate that the overall flow features are correctly captured by the present simulation as one can observe in Figs. 9 and 10. Because of the reduction of Mach number to 2.4, the angle of detached shock wave also was reduced and the temperature in the beginning of the plate is decreased. Also, one can observe that the detached shock wave moved forward of the flat plate in comparison with the first test case for free stream Mach number 4.8.

Temperature and velocity profiles along the flat plate direction is shown in Figs. 11 and 12. One can observe that the temperature distribution over the flat plate is more uniform and less sharp. In the beginning of the plate there is a heating and the temperature is around of 490 K and this value steel to the middle of the plate, when the temperature reduce abruptly to 410 K and steel reducing until to reach the value of 330 K. The velocity distribution profile is very similar to introduced before for Mach number 4.8. However, one can observe in Fig. 12 that the gradient of velocity is more smooth over the plate and one can clearly see the formation of the detached bow shock wave in front of the flat plate obstacle, as well as the flow expansion as it moves downstream of the plate.

4. CONCLUDING REMARKS

The direct simulation Monte Carlo (DSMC) method based on the molecular movement and collisions has been presented. 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 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. (4) 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. It has been shown by the present computations that the computational time required by the DSMC method increases as the Knudsen number decreases.

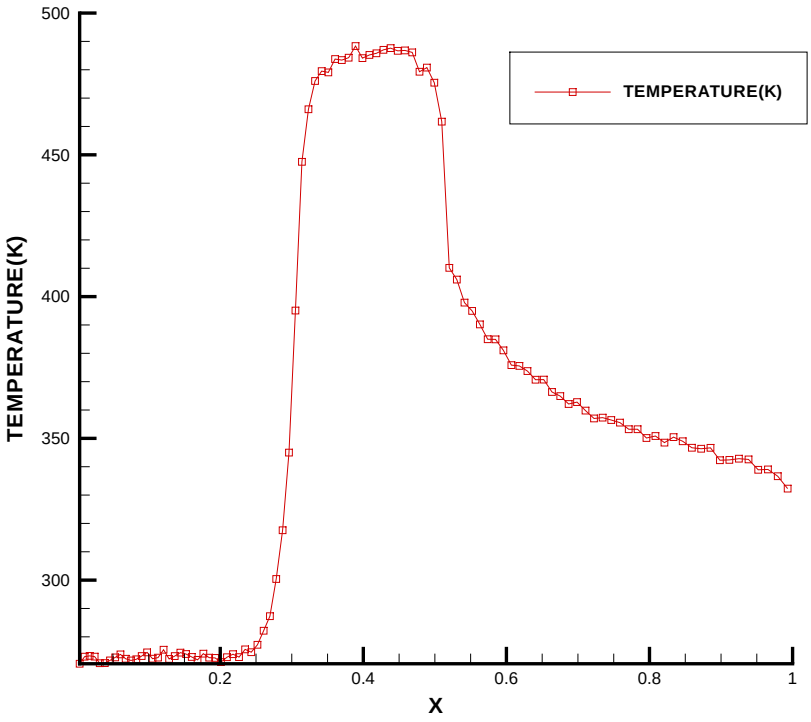

Figure 11. Temperature distribution profile throughout the flat plate configuration for free stream Mach number 2.4.

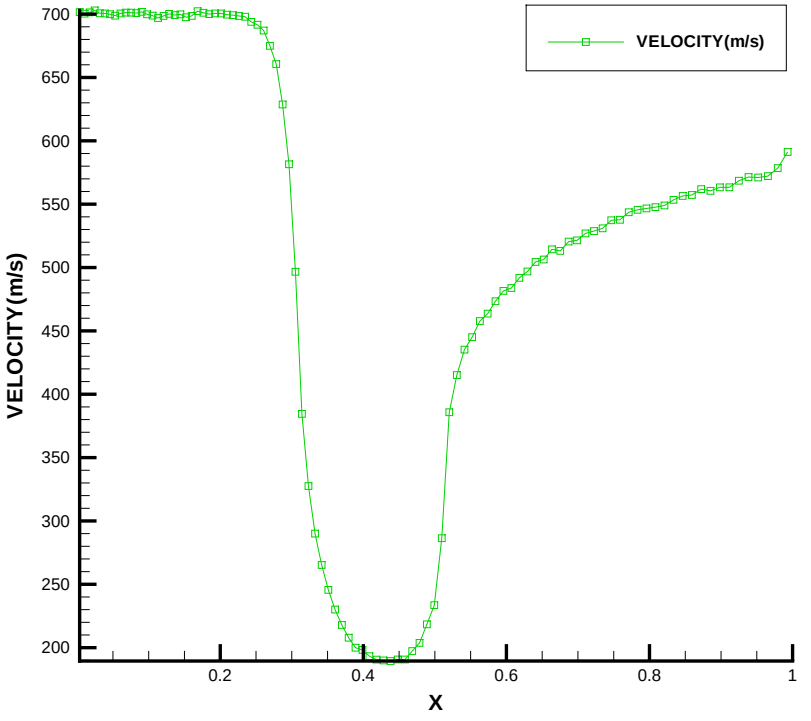

Figure 12. Velocity distribution profile throughout the flat plate configuration for free stream Mach number 2.4.

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