

All-Particle Multiscale Computation of Hypersonic Rarefied Flow

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Abstract.

This study examines a new hybrid particle scheme used as an alternative means of multiscale flow simulation. The hybrid particle scheme employs the direct simulation Monte Carlo (DSMC) method in rarefied flow regions and the low diffusion (LD) particle method in continuum flow regions. The numerical procedures of the low diffusion particle method are implemented within an existing DSMC algorithm. The performance of the LD-DSMC approach is assessed by studying Mach 10 nitrogen flow over a sphere with a global Knudsen number of 0.002. The hybrid scheme results show good overall agreement with results from standard DSMC and CFD computation. Subcell procedures are utilized to improve computational efficiency and reduce sensitivity to DSMC cell size in the hybrid scheme. This makes it possible to perform the LD-DSMC simulation on a much coarser mesh that leads to a significant reduction in computation time.

Keywords: multiscale computation, hypersonic rarefied flow, direct simulation Monte Carlo (DSMC), low diffusion – direct simulation Monte Carlo (LD-DSMC), CFD

INTRODUCTION

A hypersonic entry vehicle will experience many different flow regimes due to the change in atmosphere density with altitude. For example, the Mars Pathfinder directly entered the Martian atmosphere as an entry capsule[1,2]. It was released from the spacecraft at 130.9km and began a descent to the surface. During the descent, it experienced a wide range of flow regimes including both high and low Knudsen number regions that represent multiscale flows.

It is attractive to develop a hybrid method to analyze multiscale flows involving a wide range of Knudsen number regimes. In assessing departure from translational thermal equilibrium, a flow can be characterized by the overall Knudsen number. The flow is considered to be continuum if the Knudsen number is much smaller than one. For a Knudsen number tending to infinity, the flow regime can be considered free-molecular. The main focus in this study is the transitional regime between free-molecular and continuum regimes. If the Knudsen number is much smaller than 1, then a sufficiently large number of collisions occur for the velocity distribution to be characterized by a small departure from equilibrium, and the conventional Navier-Stokes or Euler equations are appropriate models. For this regime, continuum computational fluid dynamics (CFD) techniques may be employed to solve those equations numerically. As the Knudsen number increases, however, the continuum assumption breaks down due to the reduced collision rate, and the Navier-Stokes equations become inaccurate. At this high Knudsen number, the flow is characterized by strong thermal non-equilibrium and requires a simulation method based on kinetic theory. The kinetic simulation techniques based on the Boltzmann equation (derived from gas kinetic theory) are valid in both low and high Knudsen number regimes. The velocity distribution is determined by numerically solving the Boltzmann equation or applying a Monte Carlo method, and large deviations from an equilibrium distribution are allowed. However, these methods are very expensive to apply in the low Knudsen number regime. [3]

In recent efforts to develop schemes for simulating such multiscale flows, the most widely investigated type of method is the CFD-DSMC hybrid scheme. In an uncoupled approach, CFD calculations are applied only over near-equilibrium regions, and results from this computation are used to define inflow boundary conditions for a DSMC simulation. In a coupled approach, two very different methods (CFD and DSMC) must be integrated into a single numerical framework. However, two-way coupled information transfer between CFD and DSMC domains is complex and requires significant algorithm development.

In yet another type of hybrid approach for multiscale flow simulation, DSMC type particles are employed throughout the simulation domain. This type of fully particle approach allows simpler code development, since there

is no need to integrate two very different simulation schemes. However, particle-based equilibrium techniques are prone to large errors associated with numerical diffusion resulting from free-molecular fluxes between adjacent cells.

In the present study, the new Low Diffusion (LD) continuum particle method is used as an alternative means of low Knudsen number gas flow simulation [4,5,6]. In the LD-DSMC hybrid method, numerical diffusion errors, as well as effects of statistical scatter, are generally far smaller than in other equilibrium particle methods. This paper will discuss numerical procedures in the LD method and the application of the LD-DSMC hybrid method to hypersonic flow around a sphere.

NUMERICAL METHOD

The primary merits of the LD method are: 1) greatly reduced numerical diffusion and scatter compared with other DSMC-based methods for continuum flow simulation; 2) simple implementation in a hybrid code with DSMC; 3) inclusion of physical diffusion effects for transport coefficients that are relatively independent of cell size; along with 4) capabilities for efficient application of various DSMC models to low Knudsen number flows.

In general, the LD method is similar to the DSMC technique. A given flow domain is divided into a large number of computational cells. During each time step, particles are moved through the grid according to their assigned velocities and bulk flow properties are calculated by averaging quantities over all particles in each cell.

The main difference between LD and DSMC is related to how the velocities used for particle movement are updated during each time step. The LD method starts from the calculation of cell bulk velocity, mass density and the thermal speed for each cell. These quantities are evaluated based on cell-averaged particle values and are stored in the cell data structure. Once these properties have been determined for all cells during the current time step, a series of Lagrangian face velocities are computed. Lagrangian cells are superimposed over fixed Eulerian cells, with identical face locations at the beginning of the time step [4,5,6]. Particle positions remain fixed relative to their corresponding cell boundaries and are thus moved along with their corresponding Lagrangian cell during each time step. Particles therefore follow the macroscopic motion of Lagrangian cells, and move along trajectories that closely approximate the gas streamlines. Random particle motion associated with thermal energy is therefore greatly suppressed. As a result, numerical diffusion errors, as well as effects of statistical scatter, are greatly reduced. After each time step, particle properties are adjusted to model physical momentum and energy transport and are sorted into the Eulerian grid prior to the next time step.

To employ both LD and DSMC methods as part of a hybrid scheme, it is necessary to determine a continuum breakdown parameter that assigns appropriate allocation of cells to LD and DSMC domains. Boyd et al. proposed the use of the gradient-length local (GLL) Knudsen number [7]:

$$Kn_{GLL} = \frac{\lambda}{Q} \left| \frac{dQ}{dl} \right|$$

where λ is the mean free path, and Q is some flow quantity of interest, such as density, pressure, temperature, or velocity magnitude. In this work, LD-DSMC domain decomposition is determined based on the following GLL Knudsen number:

$$Kn_{GLL,max} = \max \left(\frac{\lambda}{\rho} |\nabla \rho|, \frac{\lambda}{T} |\nabla T|, \frac{\lambda}{a} |\nabla u| \right)$$

where ρ is the density, T is the translational temperature, u is bulk velocity magnitude, and a is the local speed of sound. Regions for which $Kn_{GLL,max}$ is larger than 0.05 are assigned to the DSMC domain, and all other regions are assigned to LD. Domain decomposition is performed once every few thousand time steps.

SIMULATION CASES

To assess the LD-DSMC hybrid method, nitrogen flow over a 12 inch diameter sphere at Mach number 10 is studied. The free stream temperature is 200 K giving a free stream velocity of 2884 m/s. The mass density is $9.875 \times 10^{-5} \text{ kg/m}^3$ and the hard sphere mean free path is $6.096 \times 10^{-4} \text{ m}$. The Knudsen number is calculated using the sphere diameter as the characteristic length. The surface of the sphere has a fixed temperature of 500K. Since axi-symmetric simulations present a difficulty to have enough particles near the stagnation point, a hybrid mesh is used in which a structured grid is employed along the forebody surface while an unstructured grid is used elsewhere in the flow field [8,9]. Three simulations are performed: (1) a standard DSMC simulation, (2) a CFD simulation

solving the Navier-Stokes equations; and (3) a LD-DSMC simulation. The simulation cases are summarized in Table 1.

TABLE 1. Simulation Cases

Cases	Number of total cells	Representative method according to the regimes	
		Continuum	Non-continuum
Standard DSMC	1,071,858	DSMC	DSMC
CFD	48,000	CFD	CFD
LD-DSMC hybrid	80,615	LD	DSMC

RESULTS AND DISCUSSION

The purpose of the present work is to validate the LD-DSMC hybrid method and to determine its computational efficiency. Based on the results that will be presented, the proposed LD-DSMC method shows good agreement with standard DSMC and CFD and achieves a high level of efficiency.

Two layers of overlapping cells are employed along the boundary between DSMC and LD domains, and are designated as buffer regions A and B. The relative locations of these buffer regions are shown in Figure 1. In buffer region A, adjacent to the DSMC domain, all simulation procedures are carried out as in DSMC cells, while in buffer region B, adjacent to the LD domain, LD calculations are performed. This provides a simple and effective means of strongly coupled information transfer between LD and DSMC domains. Here, the DSMC regions are confined to the shock wave, the boundary layer and the sphere wake flow due to the steep flow field gradients and low density found in those regions of the flow.

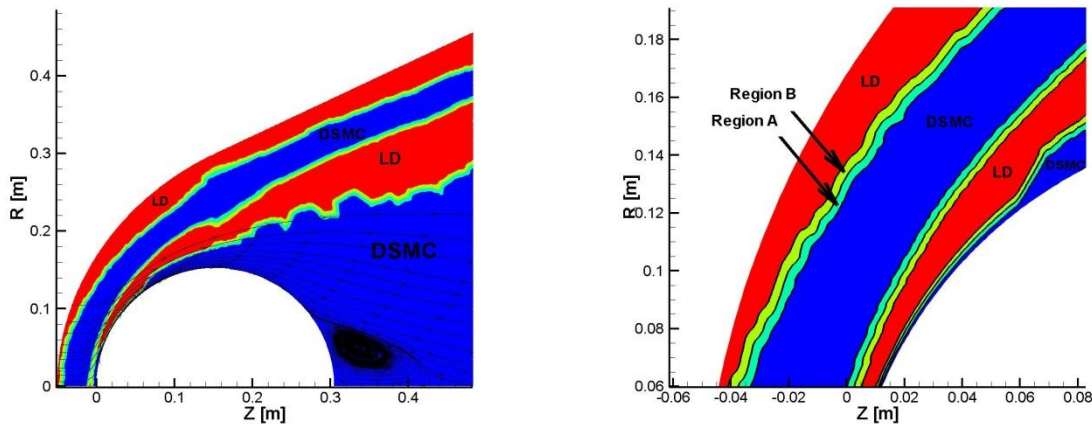


FIGURE 1. Location of DSMC and LD buffer regions in a hybrid simulation. (Right: enlargement of the left figure)

Figure 2 shows the stream lines, velocity contours and the LD/DSMC domain boundaries. Very good agreement is observed between standard DSMC, CFD and LD-DSMC hybrid results. For example, the shock standoff distance and shock shapes are nearly identical in the solutions. In the Figure 2 (left), the upper half is simulated by the standard DSMC scheme and the lower half is simulated by the LD-DSMC hybrid method. In the hybrid method, the detached bow shock is simulated in the DSMC domain, and the boundary layer near the sphere surface is also assigned to DSMC. The flow in the wake of a hypersonic blunt body involves highly rarefied conditions, so this region is also assigned as a DSMC domain. The freestream and high density post shock regions are assigned to the LD domain. In the Figure 2 (right), the upper half is simulated by standard CFD and the lower half is simulated by the LD-DSMC hybrid method. Generally, since DSMC is a particle method with accuracy in both the continuum and the rarefied regimes, it is assumed in this study that the DSMC result is most accurate. The size of the recirculation region from CFD is significantly larger than that in the DSMC and LD-DSMC results. This discrepancy indicates that the Navier-Stokes formulation becomes inaccurate in the wake, where the flow is very rarefied.

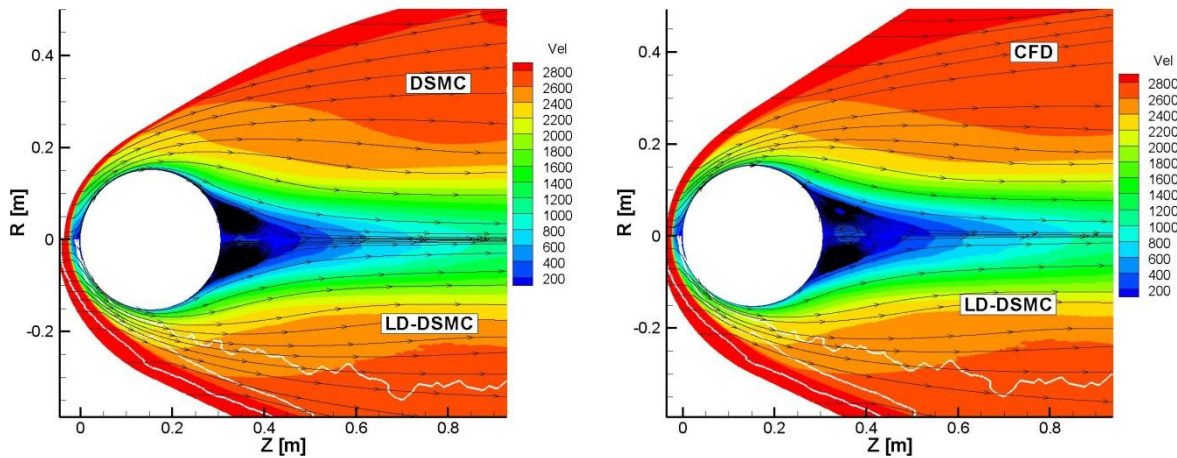


FIGURE 2. Streamlines and velocity contours from DSMC, LD-DSMC and CFD methods
(Left: upper = DSMC, lower = LD-DSMC, Right: upper = CFD, lower = LD-DSMC)

Translational temperature contours are shown in Figure 3 (left). The contours represent results from the LD-DSMC simulation; while solid lines give results from the standard DSMC computation and dashed lines represent the results of the CFD simulation. In the forebody computational domain, the DSMC result is nearly indistinguishable from the LD-DSMC result within the resolution of the figure. However, some discrepancies are obtained in the wake region. As expected, the high temperature region is focused near the forebody which has a more severe flow condition. This region is considered as key to design an effective and safe entry probe. Since the physical properties are most severe at the stagnation point, it is useful to investigate the profiles along the stagnation streamline. Profiles of the translational temperature along the stagnation streamline are shown in Figure 3 (right). The DSMC domain of the hybrid simulation includes high gradient regions within the shock. Figure 4 shows profiles of translational temperature along lines inclined at 60° and 150° from the freestream direction. In these figures, small but noticeable difference is found among the solutions. The shock is captured slightly thicker in the DSMC and LD-DSMC solutions in comparison to CFD, and the LD-DSMC simulation predicts a slightly higher temperature in the wake region.

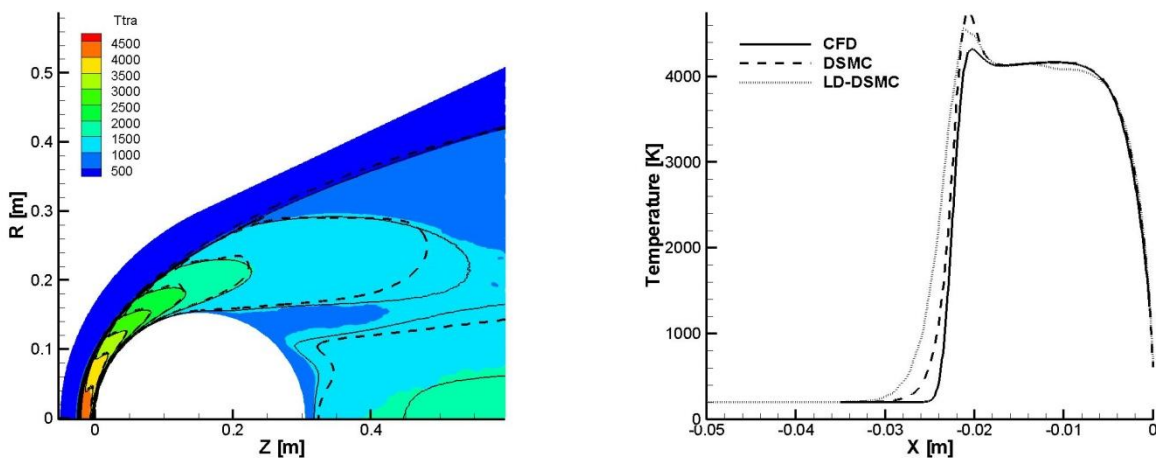


FIGURE 3. Contours of translational temperature (left) and profiles of translational temperature along the stagnation line (right)
(Contours of temperature (left): contours, solid line and dashed line represent LD-DSMC, DSMC and CFD respectively)

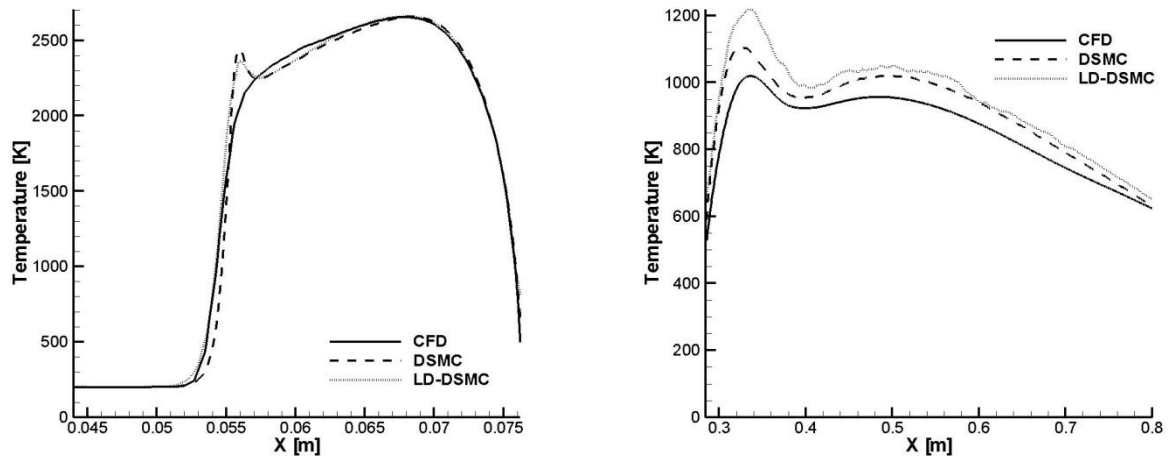


FIGURE 4. Profiles along extraction lines inclined at 60° (left) and 150° (right) from the freestream direction

Accurate prediction of surface properties is often the most important aspect of hypersonic entry problem computations for vehicle design. Figure 5 shows profiles of pressure and heat flux along the sphere surface. The pressure profiles obtained with DSMC, CFD and the LD-DSMC hybrid method show good agreement with the largest differences in the low-pressure recirculation region. The heat flux profiles show more variation particularly in the recirculation region. As mentioned above, DSMC result is most accurate and CFD (Navier-Stokes formulation) becomes inaccurate in the wake where the flow is very rarefied which explains the differences in those techniques. The hybrid simulation appears to predict higher values of both pressure and heat flux in this region and this behavior requires further study. To reduce the statistical noise, the stagnation point heat flux (DSMC, LD-DSMC) is averaged over the first ten cells along the surface. The stagnation point heat transfer coefficient and the entire body drag coefficient are calculated according to the following relations:

$$C_D = \frac{2D}{\rho V_\infty^2 S}, \quad C_H = \frac{2q}{\rho V_\infty^3}$$

The values of the coefficients are listed in Table 2, where it is shown that the present LD-DSMC results agree with standard DSMC results to within 2%.

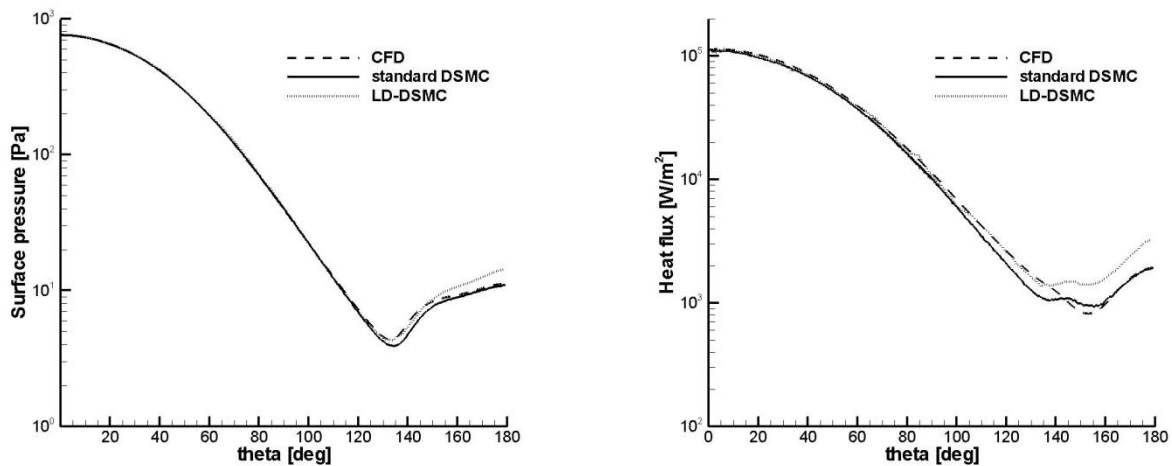


FIGURE 5. Surface pressure and Surface heat flux profiles

TABLE 2. C_H at the stagnation point, and C_D over the forebody surface

	Standard DSMC	CFD	Error	LD-DSMC	Error
C_H	0.0940	0.0971	3.3%	0.0922	1.9%
C_D	0.9629	0.9658	0.3%	0.9650	0.2%

All simulations are performed in parallel on a cluster at the University of Michigan. The LD-DSMC hybrid method shows computation expense reduction over simulations performed using standard DSMC (Table 3). A hybrid simulation is performed on a coarser mesh that provides grid independence in LD calculations, but is considerably less refined than necessary to meet DSMC guidelines [3]. During collision selection routines as part of DSMC calculations, each cell in the DSMC domain is divided into a number of subcells, with subcell dimensions set to approximately half the local mean free path. The computational cost of the LD-DSMC simulation is considerably less than the standard DSMC calculation. CFD requires less than half of the cost of LD-DSMC.

Table 3. Computation times (Kn=0.002, Ma=10)

	Standard DSMC	CFD	LD-DSMC
Speedup factor	1.0	0.05	0.12

SUMMARY

A hybrid particle scheme for the simulation of multiscale hypersonic flow has been described and assessed through comparison with DSMC and CFD simulation results. Mach 10, Kn=0.002 nitrogen flow over a sphere was used as a test case for evaluation. The results obtained with the LD-DSMC method have good overall agreement with standard DSMC that is considered the most accurate. The computational expense of the LD-DSMC hybrid simulation is reduced by a factor of 8.4 in comparison to the standard DSMC simulation primarily through the use of a coarser mesh in the continuum regions of the flow. Although LD-DSMC is more expensive than CFD, this performance suggests that the LD-DSMC scheme can compete with hybrid DSMC-CFD methods for such flows and has the additional advantage of being a simpler approach for the simulation of multiscale flows.

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