Efficient DSMC Collision-Partner Selection Schemes

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Abstract. The effect of collision-partner selection schemes on the accuracy and the efficiency of the Direct Simulation Monte Carlo (DSMC) method of Bird is investigated. Several schemes to reduce the total discretization error as a function of the mean collision separation and the mean collision time are examined. These include the historically first sub-cell scheme, the more recent nearest-neighbor scheme, and various near-neighbor schemes, which are evaluated for their effect on the thermal conductivity for Fourier flow. Their convergence characteristics as a function of spatial and temporal discretization and the number of simulators per cell are compared to the convergence characteristics of the sophisticated and standard DSMC algorithms. Improved performance is obtained if the population from which possible collision partners are selected is an appropriate fraction of the population of the cell.

Keywords: rarefied gas dynamics, Direct Simulation Monte Carlo, algorithm, hypersonic flow
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INTRODUCTION

Bird's [1-3] "sophisticated DSMC" algorithm (DSMC07) introduces several changes to the standard algorithm (DSMC94) in his 1994 monograph [4]. These changes aim at improving the accuracy and efficiency of the DSMC algorithm [3,5]. Arguably, the most important of these changes involves the scheme used to select simulators for collision. In DSMC94, collision partners are randomly selected from anywhere within a cell without regard to their separation. In DSMC07, collision partners are selected from within a cell to enforce nearest-neighbor collisions.

Assessment of nearest-neighbor selection schemes indicates [5] that their use introduces not only the potential for significant accuracy improvement but also stringent requirements for the temporal discretization. Inappropriate selection of the time step could diminish any improvement offered by these schemes by ignoring potential collision partners located along the trajectory of a simulator during the advection phase of the simulation. To remedy this, while maintaining the potential benefits of nearest-neighbor collisions, modifications to the nearest-neighbor collision-partner selection scheme that aim to improve its accuracy and efficiency have been proposed [6]. These schemes are implemented by substituting them for the nearest-neighbor scheme in the DSMC07 algorithm. In this paper, some of these schemes are reviewed and compared to the nearest-neighbor scheme in the original DSMC07 algorithm and the random-selection scheme in the standard DSMC94 algorithm.

EFFECT OF COLLISION-PARTNER SELECTION SCHEME ON CONVERGENCE

In the DSMC94 algorithm, geometrical proximity of the colliding simulators is achieved by selecting collision partners only from within the same computational cell. Thus, the mean collision separation (MCS), the average distance between two colliding simulators, is a function of the cell size and the dimensionality of the problem.

Rader et al. [7] presented a comprehensive study of the convergence behavior of the DSMC94 algorithm for one-dimensional Fourier-type flow fields. In this analysis, DSMC simulations were performed for a large number of combinations of the three discretization parameters: cell size (Δx), time step (Δt), and number of simulators per cell (N_c). Based on these simulations, Rader et al. [7] determined the dependence of the ratio of the DSMC thermal conductivity to its theoretical value as a function of the discretization parameters. A correlation for this ratio was determined using a least squares fit to DSMC results:

$$\frac{\bar{K}_{\text{wall}}}{K} = C_0 + C_{\Delta\tilde{x}^2}\Delta\tilde{x}^2 + C_{\Delta\tilde{t}}\Delta\tilde{t} + C_{\Delta\tilde{t}^2}\Delta\tilde{t}^2 + \frac{C_{N_c}}{N_c} + F\left(\Delta\tilde{t}, \Delta\tilde{x}, 1/N_c\right), \tag{1}$$

where $\Delta\tilde{x} = \Delta x/\lambda_{o,\text{HS}}$ is a dimensionless cell size ($\lambda_{o,\text{HS}}$ is the domain-midpoint value of the hard-sphere molecular mean free path), $\Delta\tilde{t} = \Delta t/t_o$ is a dimensionless time step (t_o is the midpoint mean collision time for hard-sphere molecules), and F is the contribution of higher-order powers of the discretization parameters. The values of the coefficients in Equation (1) for DSMC94 are shown in row 2 of Table 1. As theoretically predicted, a quadratic dependence of the thermal conductivity ratio to the spatial and temporal discretization parameters was observed.

TABLE 1. Coefficients of Equation (1).

$\bar{K}_{\text{wall}}/K$	C_0	$C_{\Delta\tilde{x}^2}$	$C_{\Delta\tilde{t}}$	$C_{\Delta\tilde{t}^2}$	C_{N_c}
DSMC94	1.0010	0.0405	0.0000	0.0287	-0.0830
DSMC07, TASC	0.9948	0.0048	0.0319	0.0470	0.2178
DSMC07, VSC	0.9951	0.0027	0.0629	0.0027	0.0922
DSMC07, Limit 30	0.9997	0.0017	0.0162	0.0075	-0.0881
DSMC07-D	0.9988	0.0008	0.0129	0.0129	0.0813
DSMC07-R	0.9960	0.0003	0.0121	0.0069	0.1308

Fixed sub-cells were introduced by Bird [4] to reduce the mean collision separation in DSMC simulations. In this scheme, each cell is further partitioned into smaller cells, each of which contains only a few simulators, thus reducing the MCS to a fraction of the sub-cell size. The transient adaptive sub-cell (TASC) scheme of Bird [1] is a modification of the fixed sub-cell scheme. In this scheme, cells are subdivided into sub-cells that exist only during the collision phase of each cell, and collision partners are selected from the same or neighboring sub-cells instead of from anywhere in the whole cell.

The virtual sub-cell (VSC) scheme of LeBeau et al. [9] performs an $O(N_c^2)$ operation to sort all N_c simulators in a cell to locate the nearest neighbor to any simulator chosen for collision. Since it is deterministic in selecting nearest-neighbor simulators for collisions, VSC is more accurate but more expensive computationally than TASC for large numbers of simulators per cell N_c. To assess the effect of these schemes (VSC, TASC) to the convergence behavior of DSMC, an analysis similar to that of Rader et al. [7] was presented by Gallis et al. [5]. For the Fourier problem of Rader et al. [7], Gallis et al. [5] presented correlations for the DSMC thermal-conductivity ratio for the VSC and TASC schemes that are given by Equation (1) with values shown in rows 3 and 4 of Table 1, respectively. Comparison of columns 3 and 4 of Table 1 suggests that the VSC and TASC schemes reduce the dependence on the spatial discretization by one order of magnitude compared to that of DSMC94 but introduce a first-order dependence on the temporal discretization that is not present in the original algorithm.

Based on the decrease of MCS in DSMC07 by increasing number of simulators per cell, Bird suggested that approximate nearest-neighbor collision partners, here termed near-neighbors, can be found by limiting the search to only some of the simulators in a cell (Bird suggested at most 30 selections) [2]. This limited-search VSC scheme limits the MCS reduction provided by the VSC scheme to that of 30 simulators per cell, at best, which for one-dimensional, two-dimensional, and three-dimensional flows are factors of 0.004, 0.099, and 0.201, respectively [5]. However, this limited-search VSC scheme is significantly simpler than the combination of VSC and TASC in the original DSMC07 algorithm because there is no transition between VSC and TASC. When the number of simulator selections is limited, the simulators must be randomly selected from the cell to avoid the introduction of bias.

Since the number of simulators in a cell fluctuates with time, the limited-search scheme avoids the potential degradation of performance caused by a spurious increase in the number of simulators in a cell. In particular, in cases of fixed (non-adaptive) grids and hypersonic flows, where the ratio of the local density to the free stream density may exceed two orders of magnitude near the stagnation point, not limiting the number of selections may lead to some cells spending an unnecessarily long time searching for the nearest neighbor of a simulator while gaining very little improvement in accuracy.

Using nearest-neighbor schemes in DSMC has the adverse effect of introducing a first-order temporal error in the convergence rate. The search for nearest-neighbor collision partners is physically meaningful only when the distance traveled by a simulator during a time step is smaller than the local distance between two simulators. If this condition

is violated, collision partners are selected from the vicinity of the final position of the simulator, whereas all potential collision partners along the way are ignored. This effect produces an error that is linear in the time step.

One way to mitigate this problem is not to search for the nearest neighbor of a simulator but to select a near-neighbor collision partner in the vicinity of its trajectory. In this trajectory-based scheme, the near-neighbor collision partner is selected from within a sphere centered on the simulator with a radius that is proportional to the distance traveled by the simulator during the latest advection phase. Thus, even within the same cell and with the same time step, simulators with high velocities have more simulators available as collision partners whereas simulators with low velocities have to collide with their nearest neighbor. Decreasing the radius makes the trajectory-based scheme more like DSMC07 with VSC, whereas increasing the radius makes the scheme more like DSMC94. If the radius is always large enough for all simulators in a cell to become collision partners, then the trajectory-based scheme is identical to DSMC94.

An analysis similar to that of Rader et al. [7] for the Fourier problem was conducted for the trajectory-based selection scheme. The trajectory-based scheme in which the sphere diameter is set equal to the distance traveled by the simulator is denoted DSMC07-D, and the trajectory-based scheme in which the sphere radius is set equal to the distance traveled by the simulator is denoted DSMC07-R. Thus, the sphere radius in DSMC07-R is twice the sphere radius in DSMC07-D. For the Fourier problem of Rader et al. [7], the DSMC thermal-conductivity ratios for these schemes are given by the functional form of Equation (1) with values in rows 6 and 7 of Table 1.

It is important to note that the trajectory-based selection scheme obviates the need for the stringent restrictions imposed on time step by the nearest-neighbor procedures since large time steps can be used without a significant impact on the overall discretization error of the simulation. When the collision partner selection scheme is varied for each molecule based on its individual velocity vector, larger time steps can be taken without significant degradation due to biasing the collision partners to the region near to the end of the trajectory.

FLOW OVER A 25°-55° BICONIC

The test case selected to assess the efficiency of collision-partner selection schemes is the axisymmetric flow over a 25°-55° biconic. This benchmark has been used by the NATO Research Technology Organization under the coordination of Working Group 10 [10] for a number of experimental and computational studies. This test case contains high-speed low-density regions, low-speed high-density regions, laminar expanding regions, and a laminar recirculation zone, so a DSMC simulation of this situation exercises the full spectrum of spatial and temporal conditions. The flow conditions are for the Mach 15.6 nitrogen flow experiments performed by Holden et al. [11]. The surface accommodation of nitrogen on the stainless steel surface is taken to be 0.87, as suggested by Trott et al. [12]. Nitrogen is simulated using the VSS collision model with Bird's suggested parameters [4].

The flow field is simulated with all the collision-partner selection schemes of DSMC07 presented herein. Two computational grids are used: a fine computational grid of 10^6 cells distributed so that approximately mean-free-path cell sizes are obtained, and a coarse grid of 0.25×10^6 cells constructed by coarsening the cells of the fine grid by a factor of 2 in both directions. The calculations were performed on 256 processors for the fine grid and 64 processors for the coarse grid of Glory, a 4352-processor, 272-Tflop-capable parallel computer at Sandia National Laboratories.

The convergence metric for these simulations is the size Δs of the recirculation zone, a sensitive quantity [14] in both DSMC and Navier-Stokes simulations because of the high spatial resolution that is required to resolve this feature accurately. Investigations of Moss et al. [14] indicate that the resolved size of the recirculation zone is $\Delta s_0 = 21.5$ mm and that under-resolved simulations lead to smaller Δs values, in some cases as low as $\Delta s = 16.6$ mm. Thus, the error is defined here in a normalized fashion to be $\left(\Delta s_0 - \Delta s\right)/\Delta s_0$. In the simulation results in Figure 1 (temperature and streamlines in the full domain and near the recirculation zone) and Figure 2 (heat flux on the body), calculated with DSMC07 (Case 1 of Table 2), the separation and reattachment points are at $z_1 = 79.7$ mm and $z_2 = 101.2$ mm, respectively, yielding a recirculation zone size of $\Delta s_0 = z_2 - z_1 = 21.5$ mm.

Table 2 presents the recirculation zone sizes for the biconic flow field from DSMC07 and DSMC94 simulations for six collision-partner selection schemes and the two computational grids with an average of 10 simulators per cell. Cases 1-6 use the fine grid of 10^6 cells with the indicated collision-partner selection schemes, and Cases 7-12 use the coarse grid of 0.25×10^6 cells with the same selection schemes. The symbol ∞ for the search limit denotes either finding the nearest neighbor for DSMC07 or finding either a simulator within the sphere or else the nearest neighbor for DSMC07-R and DSMC07-D. The simulation rate for each case has been normalized by the simulation rate for the first case: DSMC07 with the fine grid.

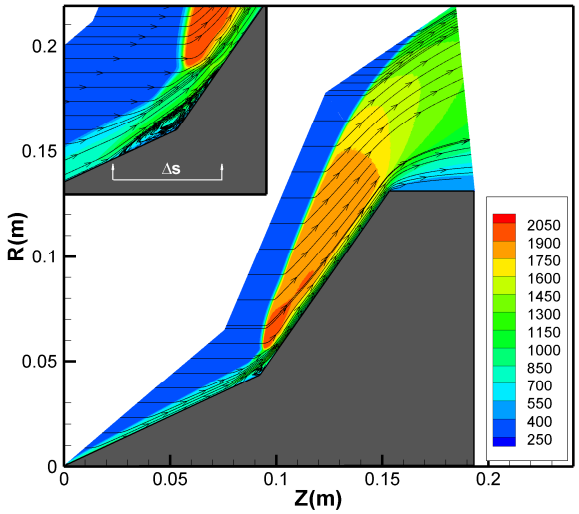

FIGURE 1. Flow field for the 25°-55° biconic.

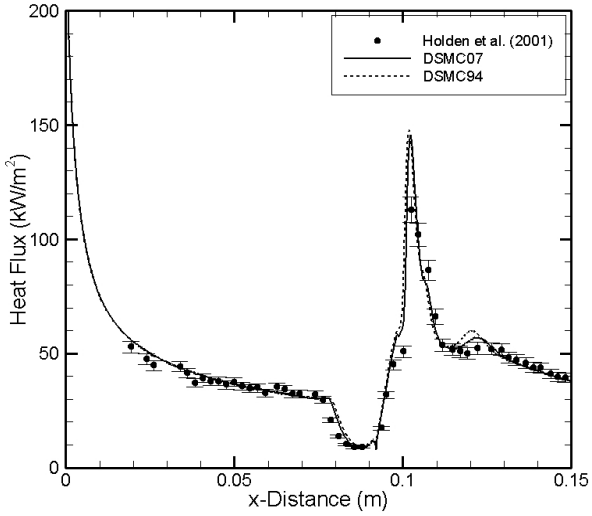

FIGURE 2. Surface heat flux for the 25°-55° biconic.

For every scheme, the recirculation zone length is predicted more accurately on the fine grid than on the coarse grid, and the amount of physical time simulated on the coarse grid is more than four times the amount on the fine grid. Reducing the search limit from ∞ to 30 to 10 to 1 (essentially DSMC94) generally increases both the simulation rate and the error, with the minor exceptions of Cases 1-2, which both produce highly accurate results. On the fine grid, all of the collision-partner selection schemes in DSMC07 (Cases 1-5) predict the recirculation zone size quite accurately (21.3-21.6 mm vs. 21.5 mm), whereas DSMC94 (Case 6) underpredicts this quantity by 6% (20.3 mm vs. 21.5 mm). For the fine grid, the simulation-rate improvements achieved by decreasing the search limit are modest: values of 1.00-1.32 are observed for Cases 1-5.

TABLE 2. Simulation rates and error for the 25°-55° biconic [11].

Case	Algorithm	Search Limit	Number of Cells	Normalized Simulation Rate	Δs (mm)	Error $(\Delta s_0 - \Delta s)/\Delta s_0$
1	DSMC07	∞	1,000,000	1.00	21.4	0.5%
2	DSMC07	30	1,000,000	1.15	21.5	0%
3	DSMC07	10	1,000,000	1.32	21.3	0.9%
4	DSMC07-R	∞	1,000,000	1.14	21.6	–0.5%
5	DSMC07-D	∞	1,000,000	1.11	21.5	0%
6	DSMC94	1	1,000,000	1.48	20.3	6%
7	DSMC07	∞	250,000	5.61	20.3	6%
8	DSMC07	30	250,000	10.8	19.8	8%
9	DSMC07	10	250,000	13.1	19.2	11%
10	DSMC07-R	∞	250,000	9.84	20.1	7%
11	DSMC07-D	∞	250,000	9.43	20.3	6%
12	DSMC94	1	250,000	9.48	16.3	24%

On the coarse grid, the effects of reducing the search limit on both the simulation rate and the error are more apparent. Notably, DSMC07-D and DSMC07 (Cases 11 and 7) both predict recirculation zone sizes of 20.3 mm, but DSMC07-D simulates nearly twice as much physical time as DSMC07. It is also important to note that, for this coarse grid, limiting the number of selections to 30 and 10 makes a non-trivial change to the size of the recirculation zone and thus to the error of the simulation.

For a fixed accuracy, the collision-partner selection scheme can significantly affect the efficiency. DSMC94 on the fine grid (Case 6), DSMC07 on the coarse grid (Case 7), and DSMC07-D on the coarse grid (Case 11) all

produce a 6% underprediction of the recirculation zone size. However, their simulation rates are 1.48, 5.61, and 9.43, respectively, so their relative efficiencies are 1, 3.79, and 6.37, respectively.

However, for the same cell size and time step, the various DSMC07 schemes have a higher computational cost than DSMC94, albeit delivering higher accuracy. Thus, in cases where the selected grid resolution can adequately resolve the flow field, the DSMC07 schemes should be limited to areas of the domain where a particular resolution is desired but not provided by the selected grid.

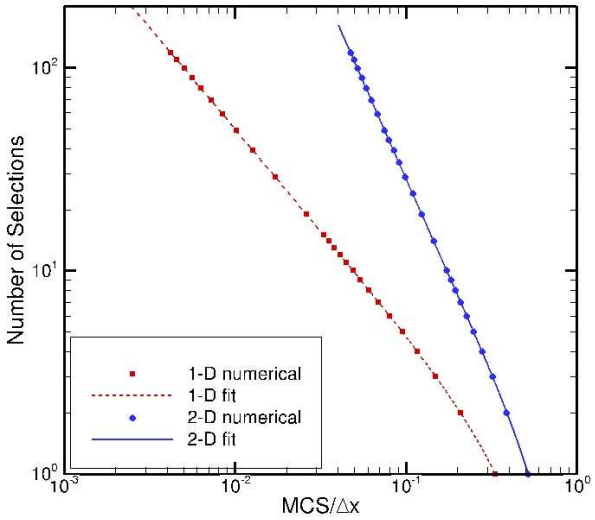

FIGURE 3. MCS reduction as a function of the number of selections.

TABLE 3. Fixed-accuracy simulation rates and error for the 25°-55° biconic [11].

Case	Algorithm	MCS/MFP	Number of Cells	Fraction of Simulation Time	Error $(\Delta s_0 - \Delta s)/\Delta s_0$
1	DSMC07-D	1.00	1,000,000	0.80	7%
2	DSMC07-D	0.50	1,000,000	0.80	8%
3	DSMC07-D	0.25	1,000,000	0.87	5%
4	DSMC07-D	0.10	1,000,000	0.93	3%
5	DSMC07-D	0.01	1,000,000	0.93	0.5%
6	DSMC07-D	1.00	250,000	0.33	18%
7	DSMC07-D	0.50	250,000	0.36	14%
8	DSMC07-D	0.25	250,000	0.38	10%
9	DSMC07-D	0.10	250,000	0.39	8%
10	DSMC07-D	0.01	250,000	0.44	6%

Instead of judiciously selecting between the two procedures, DSMC94 and DSMC07 can be combined so that they deliver the best accuracy possible at the lowest possible computational cost. The reduction of the mean collision separation as a function of the number of selections can be given as a function of the number of selections to search for the nearest neighbor, as shown in Figure 3. Using this relationship, if a particular spatial discretization is deemed sufficient, the number of selections to search for a near-neighbor can be chosen so that, provided there are sufficient simulators in each cell, the desired accuracy is achieved. Thus, only limited use is made of the highly accurate but computationally intense DSMC07 procedures.

In practice, and depending on the size of a particular cell and the number of simulators in it, the most efficient scheme (DSMC94 or DSMC07) is selected to achieve the desired accuracy. If DSMC07 is used, the number of selections to search for a near-neighbor is also decided. Thus, the DSMC07 procedures are invoked only when needed. The results for fixed-accuracy DSMC07-D simulations of the biconic for the two grids are shown in Table 3. The time needed for each method, as a fraction of the time a DSMC07-D simulation for the same grid resolution but without any limitation on the number of selections (Cases 5 and 11 of Table 2 for the fine and coarse

grid respectively), is also given. It is noted that limiting the MCS/MFP ratio allows for nontrivial time savings while the accuracy is not affected (compared to Cases 5 and 10 of Table 3). More significant time savings can also be achieved if the restriction on the MCS/MFP ratio is further relaxed (Cases 4 and 9) at a small cost in accuracy.

CONCLUSIONS

Several collision-partner selection schemes for the Direct Simulation Monte Carlo (DSMC) algorithm have been investigated, and their convergence characteristics have been compared to the convergence characteristics of the sophisticated and standard DSMC algorithms (DSMC07 and DSMC94, respectively). Essentially, each of these collision-partner selection schemes replaces nearest-neighbor collisions with some type of near-neighbor collisions.

The convergence characteristics of these schemes are studied in detail using two benchmark problems: Fourier flow and hypersonic flow over a 25°-55° biconic. Using near-neighbor collision partners rather than nearest-neighbor collision partners in DSMC07 reduces both the spatial and temporal discretization errors compared to both DSMC07 and DSMC94. However, these schemes do not change the order of DSMC07's temporal discretization error, which remains first-order, albeit small.

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