Sophisticated Versus Simple DSMC

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Abstract. The Mach 10 flow of argon past a circular cylinder at a Knudsen number 0.0091 is chosen as the test case for the comparison of results from five distinct DSMC codes. The results from all the codes are consistent, but there is a very large variation in the magnitude of the computation that has been made to obtain these results. The codes are differentiated by the extent to which they incorporate the sophisticated DSMC procedures that have been developed over the past decade. The DS2V code includes all these procedures in its default form, but most can be optionally disabled. This program is used to study the convergence of the results as the number of simulated molecules increases and as the time step decreases. While the converged values are independent of the degree to which the sophisticated procedures are activated, the rate of convergence to these values with increasing molecule number is drastically affected. The procedure that promotes nearest neighbor collisions is the most beneficial and enables a result of given accuracy to be obtained from the DS2V program with up to two orders of magnitude fewer molecules than is required by a simple DSMC program. The non-uniform time step that adapts automatically to the local mean collision time permits a given degree of time step convergence to be obtained with less than half the computational effort that is required when a fixed time step is employed.

INTRODUCTION

The MONACO DSMC code has recently been applied [1] to the hypersonic flow past a circular cylinder. The number of simulated molecules that were employed and the consequent computation time were almost two orders of magnitude higher than are required for similar calculations with the DS2V code [2]. This latter code includes several sophisticated procedures that have been developed since the 1994 publication of reference [3]. The significant difference in computational effort is relevant to two current DSMC issues:-

(i) Wagner [4] provided a convergence proof that a simple DSMC code provides a solution of the Boltzmann equation. In addition, analytical predictions of both the spatial [5] and temporal [6] discretization errors in simple DSMC have been verified by experience with these codes. The new and often complex procedures in sophisticated DSMC codes such as DS2V are not amenable to analytical study. A number of people who participated in the 2005 DSMC workshop meeting in Santa Fe expressed a preference for continuing to work with the simple procedures. The newer procedures were regarded as unproven and there were fears that they might amount to unjustifiable short cuts that could lead to erroneous results.

(ii) A variety of new methods have recently been put forward as alternatives to the DSMC method for the numerical solution of RGD flows. These methods generally incorporate physical approximations, typically a variant of BGK gas model or the lattice gas model, that are incapable of providing an accurate representation of a real gas. This deficiency is commonly justified through claims that the new method is computationally more efficient than the DSMC method. To date, there has been little attempt to base these claims on quantitative comparisons and it is important to establish the DSMC computational requirements for representative test cases.

The nominal Knudsen number 0.01 case (actually 0.0091) of reference [1] has been chosen as a test case for detailed study with the DS2V program and for comparison with whatever data is available from other DSMC codes. The diameter of the cylinder is 0.3048 m and its surface is diffusely reflecting at a temperature of 500 K. The stream velocity is 2634.1 m/s, the number density is 4.247×10^{20} /cu m, and the temperature is 200 K. The VHS model for Argon has a mass of 6.63×10^{-26} kg, a diameter of 3.595×10^{-10} m at a reference temperature of 1000 K, and a temperature-viscosity index of 0.74.

SOPHISTICATED DSMC PROCEDURES

Minimization of collision partner separation

Meiburg [7] pointed out that the simple DSMC procedures allow collisions between molecules near opposite edges of a cell and that these collisions act to destroy the angular momentum within the cell. The practical effect of this was overstated in that the preservation of any meaningful flow gradients within a cell is an advantage over most continuum methods in which angular momentum is carried only by gradients based on the grid-point values. At the same time, it was clear that the loss in angular momentum should be minimized and sub-cells [3] were introduced to that end. The gains from fixed sub-cells were limited by their adverse effect on computational efficiency and "transient sub-cells" [2] were introduced in version 3 of the DS2G program in 1998. Some early programs directly chose the nearest molecule in the cell as the collision partner for a randomly chosen molecule. This was abandoned because the computational effort was proportional to the square of the number of molecules in the cell, but was incorporated [8] into the DAC program as "virtual sub-cells". The DS2V/3V programs now employ virtual sub-cells when the number of molecules in a collision cell is less than 40 and transient sub-cells otherwise. Note that, when these "nearest-neighbor" procedures are employed, it is necessary [2] to explicitly prevent, for each molecule, successive collisions with the same collision partner. The ratio of the local mean collision separation to the local mean free path is sampled and displayed in the DS2V/3V programs and, for a good calculation, should be appreciably less than unity.

Cell structure and adaption

The number of collisions in a cell is proportional to the product of the instantaneous and average number of molecules in the cell. The average number is essentially the number density times the cell volume and commonly used collision procedures [3] make use of the sampled number density. However, if N is the instantaneous number and averages are denoted by <.>, the fact that $< N\,(N-1) >$ is identical to $< N < N > >$ in a Poisson distribution enables the collision procedures to be based entirely on the instantaneous number. This means that the DSMC procedures can be made completely independent of the sampled macroscopic properties and separate collision and sampling cells may be employed with the flow resolution being that of the smaller collision cells. Separate cells were first introduced in the SMILE program [9] and this feature is almost essential when the total number of simulated molecules is in the millions. For a given total number of simulated molecules, the quality of the results improves continuously as the number of molecules per cell decreases and values less than ten are now recommended. This means that there should be at least a million collision cells in a calculation with ten million simulated molecules and this would be impractical if it meant that there were also more than a million sampling cells. A small and uniform number of molecules per collision cell can be achieved only by adapting these cells to the flow. The quality of the output is improved if the sampling cells are also adapted to a uniform sample size per cell. In addition, because the number of collision cells is very large, it is not practical to follow the molecules from cell to cell by calculating intersections with cell boundaries and the geometry model must allow the direct determination of the cell from the molecule coordinates. In addition to satisfying these conditions, the DS2V/3V geometry model [2] scales trivially from two to three dimensions.

Time step adaption

For a good calculation, the time step must be small in comparison with the mean collision time and simple programs employ a user specified time step that is uniform over the flowfield. The ratio of the maximum to the minimum value of the mean collision time in the cylinder test case is just over one hundred. If a uniform time step is sufficiently small in comparison with the minimum mean collision time near to the stagnation point, it is excessively small over the remainder of the flowfield. This leads to an inefficient calculation and most existing calculations of cold surface hypersonic blunt body flows with simple DSMC codes have employed time steps that are too large in the vicinity of the stagnation point. The solution is to employ a variable time step that adapts everywhere to a specified fraction of the sampled local mean collision time. The procedures to do this in the DS2V/3V codes require the assignment of a time parameter to every molecule and to every cell.

Automatic setting of the computational parameters

The automatic adaption of the time step relieves the user of the difficult task of setting the time step. Most of the other computational parameters can also be set automatically and the only parameter that must be set by the user in the DS2V/3V programs is the initial number of megabytes to be used by the calculation

COMPARATIVE RESULTS

DSMC and continuum results were compared in reference [1] primarily through the overall drag and the net stagnation point or peak heat transfer. The drag is one of the quantities that are least sensitive to the computational parameters, while the heat transfer is one of the most sensitive. The net heat transfer is particularly challenging if the incident and reflected heat fluxes are near equal but, in this case, the value of the reflected flux is just half that of the incident flux. The results for these quantities from the DSMC programs that have already been mentioned in this paper are shown in Table 1.

Program	Total Simulated Molecules	Total Cells	Time Step (μ sec)	Computation Time (hours)	Drag (N)	Peak Heat Transfer (W/sq m)
MONACO	26,800,000	34,770	0.02	1872 parallel CPU	40.00	39,319
DS2G (ver. 2)	2,900,000	129,600 (sub-)	0.2	20 on 3GHz PC	39.95	38,300
SMILE	24,000,000	4,000,000 (coll.)			39.76	39,000
DAC	1,300,000			15 on 3GHz PC	39.71	38,500
DS2V	330,000	41,000 (collision)	0.12 (min.)	10 on 3GHz PC	39.76	38,400

TABLE 1. .Results for the hypersonic cylinder test case from five DSMC codes.

The spread in the results is 0.7% for the drag and 2.6%.for the peak heat transfer. This is reasonably good, although several results lie outside the range of variation that would be expected to be produced by statistical scatter and different stages of convergence with regard to the spatial and temporal resolution of the flow. All calculations were made for a half cylinder with a plane of symmetry parallel to the flow direction through the axis of the cylinder. Most calculations set the origin at the stagnation point and the upstream downstream and outer boundaries at -0.2 m, 0.65 m, and 0.4 m. The flowfield was larger in the SMILE calculation and the DS2V run was repeated with this larger flowfield. The DS2V values did not change and the heat transfer distributions are compared in Fig. 1. A logarithmic scale has been used to bring up the excellent agreement in the downstream region of the flow. A small vortex extended over the final three or four sampling intervals.

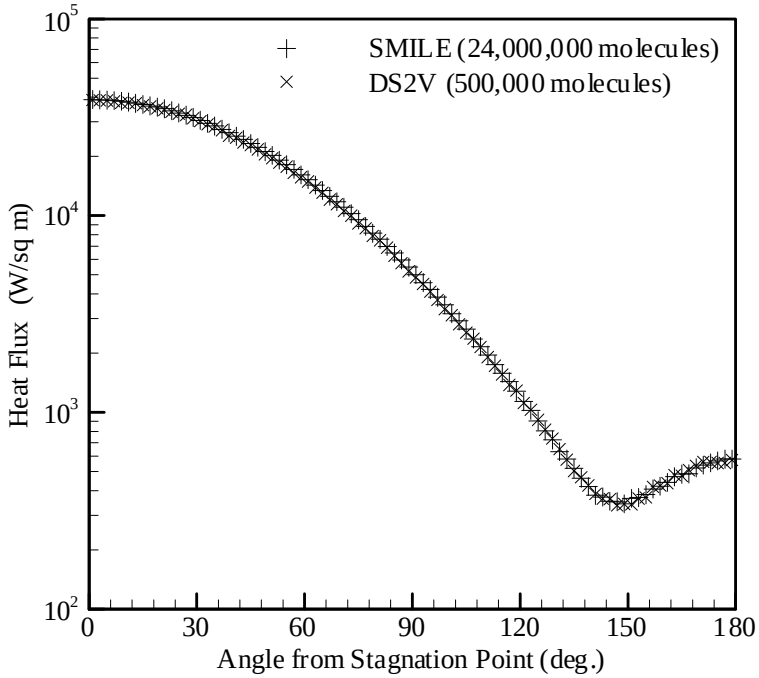

FIGURE 1. The distribution of heat transfer around the cylinder.

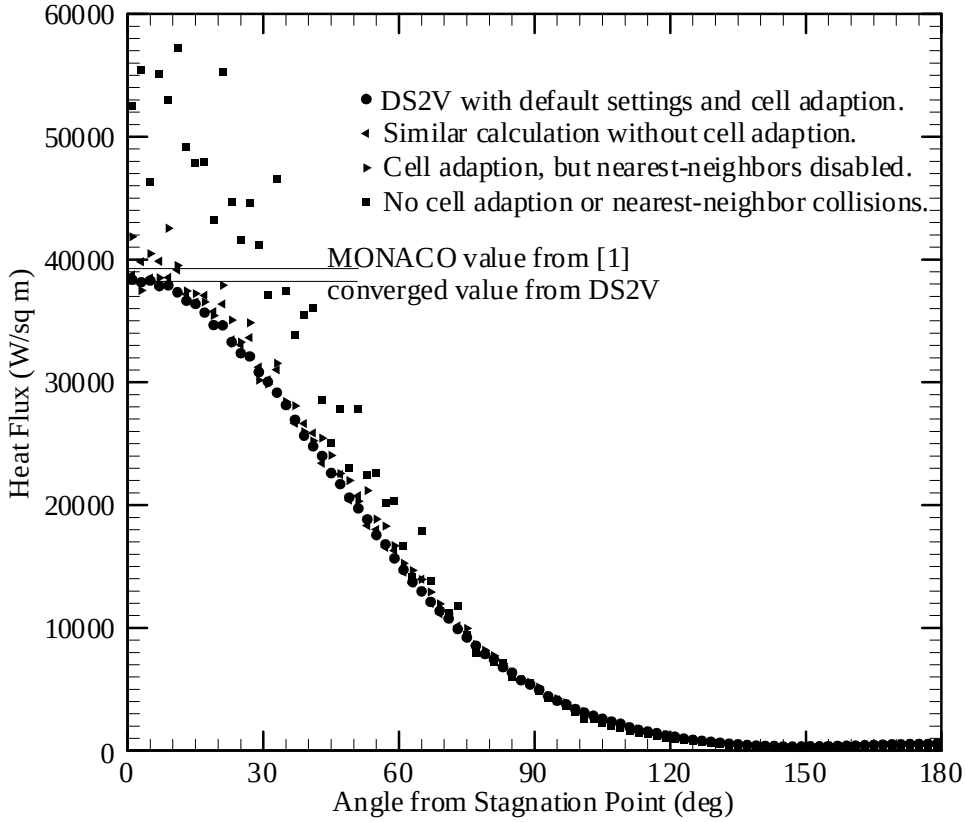

FIGURE 2. The influence of the sophisticated procedures in DS2V calculations with 330,000 simulated molecules.

The nearest-neighbor procedures in the DS2V program may be disabled and the runs can, of course, be made with or without default cell adaption. Figure 2 compares the DS2V case* from Table 1 with similar runs in which one or both procedures have not been employed. The absence of a single procedure leads to a degradation in the results and that due to the disabling of the nearest-neighbor procedures is the more serious. A surprising result is that the combined error is far greater than the sum of the individual errors. Moreover there is a qualitative as well as a quantitative degradation of the profiles. All runs were of similar magnitude with a sample of more than 600,000 molecules striking each surface interval near the stagnation point and the statistical scatter should be similar in all runs. A sample of the order of 100,000 is adequate for an engineering calculation and, because the steady state is reached in less than one hour, this requires only three hours on a contemporary PC.

DS2V CONVERGENCE STUDIES

Figure 3 shows that the relationships between the results from the four options change as the total number of simulated molecules is varied. Except for very small molecule numbers when the default adaption leads to a reduction in the number of collision cells, there is an improvement after cell adaption. This is most pronounced when the nearest-neighbor procedures are disabled. With cell adaption, the nearest-neighbor procedures lead to a near-converged result with less than a tenth the number of molecules that are required when these procedures are disabled. The number of molecules that are required for a near-converged result in an adapted DS2V run is less than one percent of the number required in an unadapted run with the nearest-neighbor procedures disabled.

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* This is also Demonstration Case # 9 in the DS2V code that is available as a free download from gab.com.au and can be run on any Windows PC.

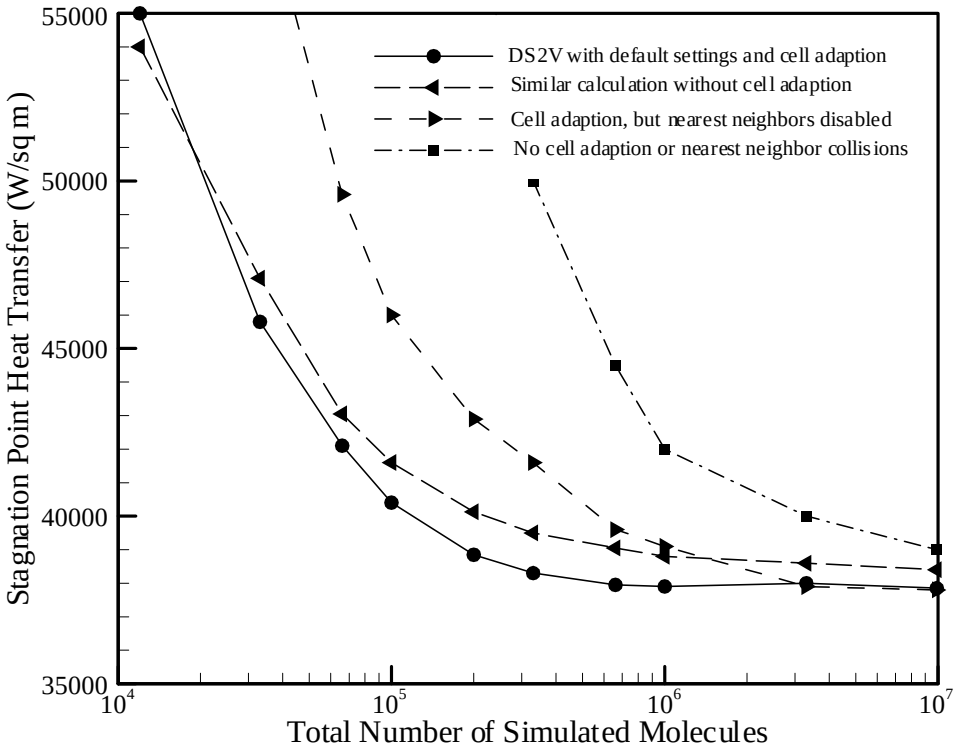

FIGURE 3. Convergence with molecule number in DS2V runs with the default time step.

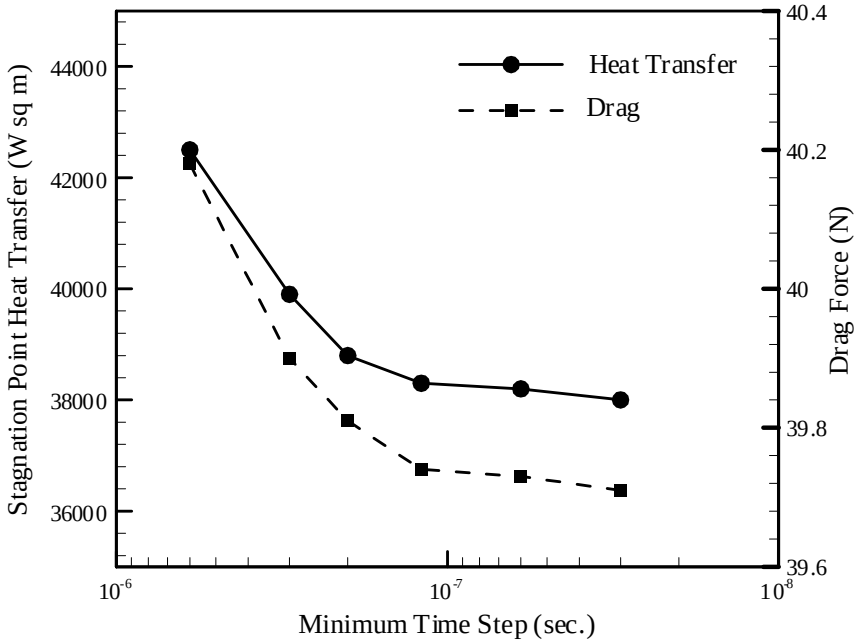

FIGURE 4. Convergence with minimum time step in DS2V runs with 330000 molecules.

A significant result with regard to the validity of the nearest-neighbor procedures is that they have no effect on an adapted flow when the total number of molecules exceeds three million. However, if they are not employed, there are large changes in the flowfield when adaption occurs. These changes produce significant transient disturbances that lead to a temporary reduction in the peak heat transfer by as much as ten percent.

The default DS2V time step is one third the local mean collision time. This can be varied between one fifth and one half the mean collision time each time that a run is restarted. The minimum value with the default setting and 330,000 simulated molecules is 1.2×10^{-7} seconds. Figure 4 shows that this leads to a near-converged result. For a variation in time step through a factor of twenty, the drag changes by 1.2% and the peak heat transfer by 11%. The mean value of the time step is three times the minimum value and, allowing for overheads, the variable time step increases the computational efficiency by a factor of more than two.

The DS2V interactive display includes advice to the user on the number of molecules that are required for a good calculation. This is based on the sampled ratios of the mean collision separations to the local mean free path. The advice for this problem proved to be unduly pessimistic. When convergence with regard to both molecule number and time step is taken unto account, the DS2V result for the peak heat transfer is 37,600 ± 200 W/sq m and that for the drag is 39.68 ± 0.05 N.

CONCLUDING REMARKS

For this problem, the sophisticated DSMC procedures do not lead to error and can reduce the number of simulated molecules that are required to obtain a result of given accuracy by two orders of magnitude. The computation time is not reduced to anything like the same extent because a longer run is needed to obtain the same sample size. However, in addition to the statistical scatter associated with the sample size, there is also a systematic unevenness in the results that is minimized by the sophisticated procedures. In addition, the reduction in the required number of simulated molecules leads to a reduction in the fraction of the run time that is occupied by the unsteady phase of the flow and by any transients caused by flow adaption.

The sophisticated DSMC procedures increase the memory requirements, but this increase is small in comparison with the memory that is saved by the reduction in the required number of simulated molecules. For a given computer, the sophisticated procedures enable calculations to be made at much lower Knudsen numbers. This hypersonic cylinder test case at Kn = 0.0091is an easy calculation on a contemporary PC. It is still far from a continuum calculation because the maximum slip velocity exceeds 200 m/s and the maximum temperature slip exceeds 300K. Continuum flow would require a reduction in Knudsen number by a factor of about five and this would be beyond the capabilities of a PC if the sophisticated procedures were not employed.

These conclusions apply only to the single test case. Additional problems and test cases should be studied in similar detail in order to build a database of validated results. The relative merits of various DSMC codes and of new methods that are proposed as alternatives to DSMC could then be assessed through quantitative rather than qualitative comparisons.

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