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An Improved-Efficiency DSMC Algorithm

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Abstract. The Direct Simulation Monte Carlo (DSMC) method has been repeatedly criticized for its computational efficiency in comparison with the less accurate, but computationally efficient, continuum methodologies. Recently, and in response to this criticism, the originator of the method proposed a new variant of DSMC, termed "sophisticated DSMC". This new DSMC algorithm aims at improving the computational efficiency of DSMC without losing the accuracy of the original algorithm. In this paper the accuracy and convergence of the new DSMC method are investigated for one-dimensional combined Couette-Fourier flow. The primary convergence metrics studied, in harmony with previous work, are the ratios of the DSMC-calculated thermal conductivity and viscosity to their corresponding infinite-approximation Chapman-Enskog theoretical values. As discretization errors are reduced, the DSMC values are shown to approach the theoretical values to high precision. The convergence behavior of sophisticated DSMC is compared to that of standard DSMC and to predictions of Green-Kubo theory. The sophisticated algorithm is shown to significantly reduce the computational resources required for a DSMC simulation at a fixed level of accuracy.

Keywords: DSMC, sophisticated DSMC, algorithm, convergence, accuracy, rarefied gas dynamics
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INTRODUCTION

Since originally proposed more than 40 years ago, the Direct Simulation Monte Carlo method [1] has no rivals for practical non-continuum rarefied-gas-dynamics calculations. Despite being more efficient than any other numerical technique with the same capabilities, the algorithm has been repeatedly criticized for its computational efficiency in comparison with the less accurate, but computationally efficient, continuum methodologies.

In response to this criticism, Bird has recently proposed a new variant of DSMC, termed "sophisticated DSMC" [2,3]. This new DSMC algorithm aims at improving the computational efficiency of DSMC without losing the accuracy of the original algorithm. To achieve this, significant modifications to the way molecules move and collide are introduced. More efficient grids and adaptive time steps that vary across the domain are used to gain computational efficiency during the move phase. In the collision phase, the new algorithm abandons the random selection of collision partners within a cell in favor of a nearest-neighbor selection scheme. All these modifications aim at optimizing critical simulation parameters at a relatively low cost, leading to an enhanced DSMC algorithm.

In this paper, the ability of the sophisticated DSMC algorithm to deliver improved computational efficiency while maintaining its unprecedented accuracy in simulating gas flows is examined. The benchmark cases used for this purpose are Fourier and Couette flow. More than 500 simulations covering the regime from near-equilibrium to non-equilibrium conditions are performed. The results of the sophisticated DSMC method are compared with those of the traditional method for the same problem. Herein, DSMC07 and DSMC94 (i.e., as published in Bird's 1994 monograph [1]) are used to distinguish the sophisticated and traditional DSMC algorithms.

A NEW DSMC ALGORITHM

The sophisticated DSMC07 algorithm retains the basic elements of the DSMC94 algorithm described in Bird's monograph [1]. The key computational assumptions of DSMC, the uncoupling of molecular motion and collisions over small time steps and the partitioning of the physical domain into small cells, are maintained. The modifications to the algorithm mainly involve changes to the ways that molecules are selected for collisions and that collisions are distributed over the duration of a time step. Besides the global time that a DSMC code keeps track of, molecule-based and cell-based times are calculated and kept track of as well. To achieve this, the DSMC07 global time is advanced in small global time steps that are typically a small fraction of the time step used by a DSMC94 code. Unlike the DSMC94 algorithm, only a small fraction of the molecules move and collide at any global time step.

The introduction of sub-cells in DSMC simulations was the first attempt to improve the accuracy of the simulation algorithm without excessive storage or time penalties due to the very large number of fine cells. It was subsequently realized that the memory cost of the sub-cell scheme could be reduced if the sub-cell structure is considered only during the collision phase by employing a temporary sub-cell structure that is created at each time step when the cell is considered for collisions. This scheme, termed the *transient-adaptive sub-cell* technique, was originally implemented by Bird in the DS2V [3] series of codes as part of the DSMC07 algorithm, and it aims at a single-molecule per sub-cell structure. The memory penalty of this scheme is minimal because the sub-cell structure is created only for a single cell, the cell being considered for collisions. After the end of the collision phase for the particular cell, the information about particle indexing is discarded.

The idea of performing an N^2 operation to sort all N molecules in a cell was initially considered unacceptably expensive to be implemented. LeBeau [4] demonstrates that, for a small number of simulators per cell (~10), this technique, termed the *virtual sub-cell* technique, could actually provide an efficient way of performing collisions minimizing the mean collision separation. Nearest-neighbor selection was then implemented in Bird's DS2V/3V [3] codes as part of the sophisticated DSMC algorithm and was found to be faster than transient-adaptive sub-cells when the number of molecules per cell is less than a number between 30 and 40.

The virtual sub-cell and transient-adaptive sub-cell techniques are the two alternatives of DSMC07 collision partner selection. Being deterministic in selecting nearest-neighbor molecules, the virtual sub-cell technique is more accurate but also more expensive computationally. Because it selects nearest-neighbor molecules in a probabilistic manner, the transient-adaptive sub-cell technique is less accurate, but it is computationally more efficient. Bird recommends the virtual sub-cell technique for cells with up to 30 simulators and the transient-adaptive sub-cell technique for cells with more than 30 simulators.

The use of a single fixed time step becomes inefficient when the ratio of maximum to minimum density becomes large. In flow fields where there are significant variations of the local collision time, this requires a time step that varies over the flow field and adapts automatically to the local mean collision time and/or, for high-Knudsen-number flows, to the transit time of molecules through the cell. In contrast with the DSMC94 algorithm, which uses the same time step throughout the domain, a variable time step is introduced by continuously updating a desired time step (DTS) in every collision cell. This time step for a collision cell is set to the minimum of a specified fraction of the local mean collision time and a specified fraction of the transit time for that cell. A time parameter is assigned to every molecule and to every collision cell. The flow time is advanced in steps equal to the smallest value of DTS. Then, if the time parameter of a molecule falls behind the flow time by DTS/2, the molecule moves a distance corresponding to DTS, and the molecule's time parameter is increased by DTS. Similarly, if the time parameter of a collision cell falls behind the flow time by DTS/2, collisions are performed in that cell over the time interval DTS, and the cell's time parameter is increased by DTS. Practically, this results in a background global time step that is about 5-10 times smaller than the cell time step.

It should be pointed out that in DSMC94 the error due to temporal discretization arises from the fact that collisions are performed at discrete times between the move operations although collisions actually occur continually throughout time. The sophisticated approach mitigates this problem somewhat because collisions in a cell are spread over the duration of a time step, which allows for a more physically realistic simulation.

DSMC SIMULATIONS

For small system and gradient Knudsen numbers, Chapman-Enskog (CE) theory [5] provides accurate predictions for the transport properties and velocity distribution functions established in the bulk gas. Since CE predictions are used to assess the accuracy of the DSMC94 algorithm [6,7], the same comparisons are performed for the new DSMC07 algorithm. Following previous work [6,7], a gas that has the molecular mass and the reference viscosity of argon is considered. The Maxwell and hard-sphere interactions bracket the interactions of most known molecules and thus are examined. The Variable Soft Sphere (VSS) model is used to represent these interactions: Maxwell molecules have $\omega = 1$ and $\alpha = 2.13986$, and hard-sphere molecules have $\omega = 1/2$ and $\alpha = 1$. Initially, the gas is motionless and at the reference pressure and temperature: $p_{\text{init}} = p_{\text{ref}} = 266.644$ Pa (2 Torr) and $T_{\text{init}} = T_{\text{ref}} = 273.15$ K. The domain has a length $L = 1$ mm and is bounded by two parallel solid walls that reflect all molecules diffusely at the wall temperature (unity accommodation). The system Knudsen number at the initial conditions is $\lambda/L = 0.0237$, so the walls are about 42 mean free paths apart.

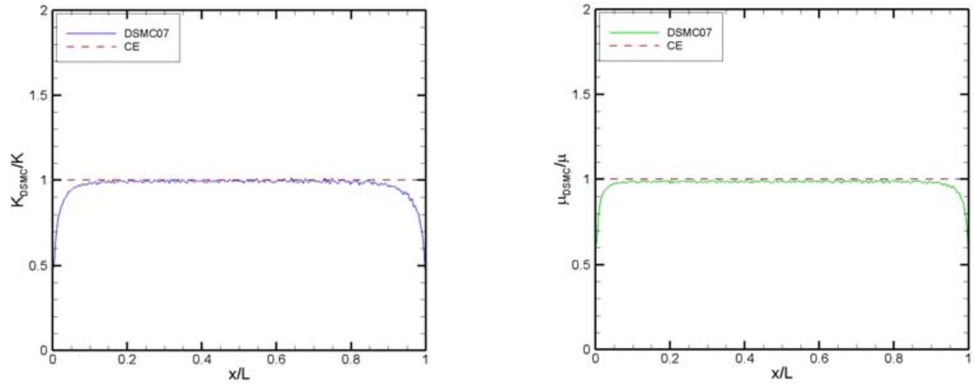

FIGURE 1. Profiles of thermal-conductivity ratio (left) and viscosity ratio (right) for Maxwell molecules.

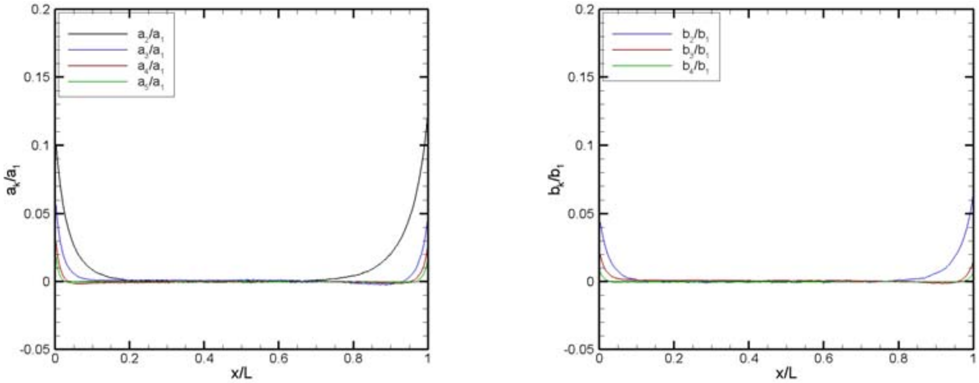

FIGURE 2. Sonine-polynomial-coefficient profiles for Maxwell molecules: left, a_k/a_1; right, b_k/b_1.

Figure 1 shows the normalized thermal-conductivity and viscosity profiles for Maxwell molecules at these conditions as a function of the distance between the two plates. The effective values K_{DSMC} and μ_{DSMC} are determined using the DSMC temperature, velocity, heat-flux, and shear-stress profiles as in the earlier study [6]. The transport properties are normalized using the corresponding CE values. A value of unity indicates that the CE value is obtained, which occurs in the central region of the domain. The Knudsen layers are restricted to about 10-25% of the domain adjacent to each wall. The heat-flux and shear-stress Knudsen numbers [6,7] at these conditions are $\text{Kn}_q \approx 0.006$ and $\text{Kn}_\tau \approx 0.003$, respectively, and thus are quite small, so CE theory applies in the central region of the domain, and departures are observed only in the Knudsen layers adjacent to the walls.

Figure 2 shows the corresponding profiles of the Sonine-polynomial-coefficient ratios a_k/a_1 and b_k/b_1 [6,7]. As observed for the thermal conductivity and the viscosity, the Sonine-polynomial-coefficient ratios achieve the CE values in the central region of the domain and depart from the CE values only in the Knudsen layers. Similar agreement is found for other molecular potentials [8].

Under highly non-equilibrium conditions, the CE theory discussed in the previous section is no longer applicable and is superseded by the Moment-Hierarchy (MH) method. The MH method is useful for Maxwell molecules because the collision rate for the Maxwell interaction is independent of the molecular relative speed. Thus, for Maxwell molecules, the MH theory gives expressions for the thermal conductivity, the viscosity, and the Sonine-polynomial-coefficient ratios in terms of the heat-flux and shear-stress Knudsen numbers.

To investigate the non-equilibrium regime, Fourier-Couette flow is used again, but in this case the temperature difference is increased so that non-continuum effects in the bulk gas are no longer small. All other parameters used in the previous example are kept the same. Thus, the walls have temperatures $T_1 = T_{\text{ref}} - \Delta T/2$ and $T_2 = T_{\text{ref}} + \Delta T/2$

and tangential velocities $V_1 = -\Delta V/2$ and $V_2 = \Delta V/2$ with temperature differences up to $\Delta T = 400\ \mathrm{K}$ and a velocity difference of $\Delta V = 100\ \mathrm{m/s}$. Within the central region, the variation of the a_k/a_1 and the b_k/b_1 with Kn_q represents the normal solution to the Boltzmann equation. Since the heat-flux Knudsen number Kn_q varies across the domain, a single DSMC simulation provides the normal solution for the range of Kn_q values in the central region.

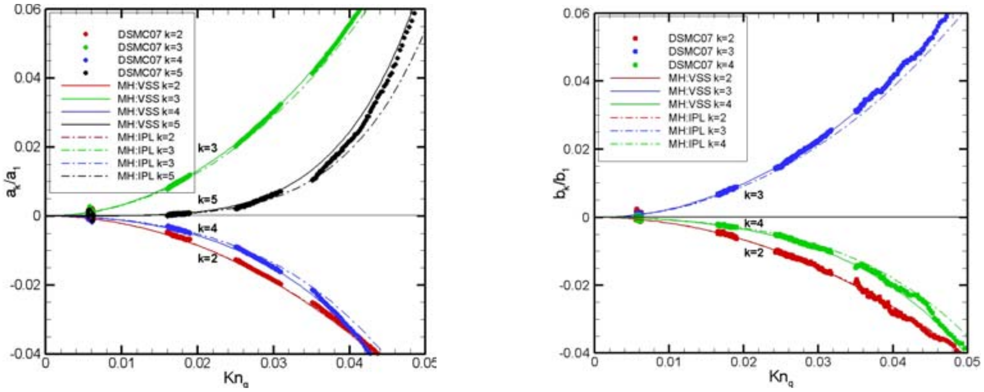

FIGURE 3. Sonine-polynomial coefficients for Maxwell molecules: left, a_k/a_1; right, b_k/b_1.

Figure 3 shows the a_k/a_1 and the b_k/b_1 for Maxwell molecules as functions of Kn_q. The symbols indicate the DSMC07 values. Each cluster of points along a curve corresponds to values obtained from the central region of a single DSMC simulation with temperature differences of $\Delta T = 70,\ 200,\ 300,\ 400\mathrm{K}$ and a velocity difference of $\Delta V = 100\ \mathrm{m/s}$. In all cases, the shear-stress Knudsen number Kn_τ is below 0.005, which classifies the flow as in the continuum-hydrodynamic regime as far as shear stress is concerned. The solid and long-dashed curves are the corresponding MH results for VSS-Maxwell and IPL-Maxwell interactions [6,7].

The DSMC07 values agree closely with the MH VSS-Maxwell values except for a_4/a_1 and a_5/a_1 at $\Delta T = 400\ \mathrm{K}$ (the largest temperature difference). A similar difference between DSMC94 and theory is attributed to discretization errors and to the small but finite Kn_τ. The DSMC07 and MH results for the VSS-Maxwell interaction are in good agreement, which provides strong evidence that DSMC07 produces the correct velocity distribution function. It is noted that the a_k/a_1 and the b_k/b_1 differ appreciably from the CE values when $\mathrm{Kn}_q > 0.01$.

CONVERGENCE OF DSMC07

To evaluate the effect of the proposed changes to the DSMC94 algorithm, the analysis of Rader et al. [9] is repeated with the DSMC07 algorithm. By using the same test case (pure Fourier flow with a hard-sphere argon-like gas), not only can the convergence behavior of the new algorithm be derived, but also a direct comparison between DSMC07 and DSMC94 can be performed at the same time.

More than 500 simulations are performed where the basic simulation parameters, number of simulators per cell, time step, and cell size, are systematically varied. The simulations use a normalized parameter space bounded by $0.01 \le 2\Delta\tilde{t} \le 1$ for the time step, $0.105 \le \Delta\tilde{x} \le 2$ for the cell size, and $5 \le N_c \le 120$ for the number of simulators per cell. The thermal-conductivity ratio is calculated as a spatial average over the central part of the domain as in Rader et al. [9]. Each calculation involved ensemble-averaging of 100 realizations of the same problem initialized with different seeds for the random-number generator. These 100 realizations are averaged over the number of independent runs. To compare with the results of the one-dimensional DSMC94 code [7], the virtual sub-cells (nearest-neighbors) are selected based on their x distance only.

Figure 4 presents the results for 15 simulators per cell. In these figures, the dot-dashed curves represent the convergence behavior of DSMC94, as given by Rader et al. [9], the solid symbols represent DSMC07 calculations for the same cases, and the solid curves are the least-squares fit to the DSMC07 results, given below:

$$\begin{aligned}\frac{\bar{K}_{\mathrm{DSMC07}}}{K} = {} & 0.995084 + 0.0628887\Delta\tilde{t} + 0.0477988\Delta\tilde{t}^2 + 0.00267194\Delta\tilde{x}^2 - 0.00335372\Delta\tilde{t}^4 \\ & + 0.00193386\Delta\tilde{t}^2\Delta\tilde{x}^2 - 0.106218/N_c^2 + 0.092157/N_c + F(\Delta\tilde{x},\Delta\tilde{t},1/N_c)\end{aligned}. \qquad (1)$$

Figure 4 presents the convergence behavior of the thermal-conductivity ratio both as a function of cell size and as a function of time step. In harmony with the observations for an infinite number of simulators, the thermal-conductivity convergence rate is less sensitive to the spatial discretization for DSMC07 than for DSMC94. The opposite is true for convergence behavior as a function of the temporal discretization because of the strong influence of the linear $\Delta\tilde{t}$ term in Equation (1).

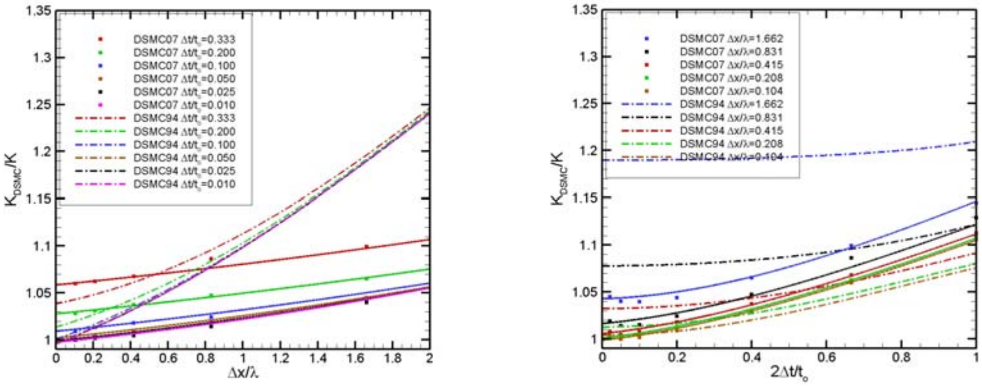

FIGURE 4. Thermal-conductivity ratio for $N_c = 15$ as a function of $\Delta\tilde{x}$ (left) and $\Delta\tilde{t}$ (right).

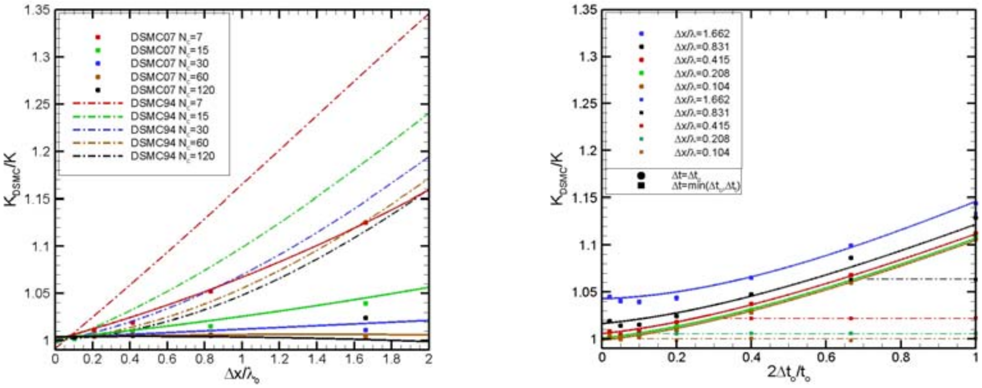

FIGURE 5. Left: thermal-conductivity ratio for $\Delta\tilde{t} \le 0.10$ MCT as a function of $\Delta\tilde{x}$ and N_c.
Right: thermal-conductivity ratio for $N_c = 15$ as a function of $\Delta\tilde{t}$ with $\Delta\tilde{t} \le 0.25$ MTT .

Comparison of these figures indicates that, in the limit of vanishing discretization error, both methods converge to the correct answer of unity to within fitting uncertainty. For coarser discretization, DSMC07 produces a smaller error in general. The cell size clearly plays a much smaller role in determining the error in DSMC07 simulations. In fact, the DSMC07 error is always smaller when the time step is smaller than the mean collision time and the cell-transit time. It appears that using time steps greater than the mean collision time or allowing molecules to bypass cells without examining them for potential collision partners violates the principle of the nearest-neighbor method. Assuming that the motion of a molecule is contained within a cell, by allowing molecules to travel further than one mean collision separation, the nearest-neighbor scheme biases collisions to molecules in the vicinity of the final position, ignoring all molecules between the initial and final positions. The DSMC94 algorithm, by disregarding the location of the molecules in the cell, allows all molecules to be considered.

To further demonstrate this point, the left plot in Figure 5 presents results for which the time step is constrained to be 1/4 of the mean transit time (MTT) as well as a fixed fraction of the mean collision time (MCT), as proposed by Bird [3]. In this case, the DSMC07 error is always smaller than the DSMC94 error.

A better representation of the improved performance of the new method is given in the right plot of Figure 5, which present the convergence behavior as a function of the cell size for multiple values of the number of simulators per cell. For a particular number of simulators per cell and for small enough time steps, the DSMC07 error is smaller than the DSMC94 error. The effective time step of the calculations presented in the right plot of Figure 5 (7 ns) is such that molecules cannot travel more than one cell.

The above comparisons point out the stronger role that temporal discretization plays in DSMC07 than in DSMC94. This can be explained by a violation of the assumptions behind the nearest-neighbor selection scheme. The adoption of the nearest-neighbor method recognizes the importance of not overlooking neighboring simulators when collision partners are selected. A time step that is larger than the mean collision time would result in molecules traveling past potential collision partners without their ever having the chance to be selected for collision. This behavior is described by the linear convergence rate of the thermal-conductivity ratio with time step.

For small numbers of simulators per cell, additional error sources seem to become more important due to the $1/N_c$ and $1/N_c^2$ terms, making the convergence behavior more complicated. It is noted that DSMC07 has positive $1/N_c$ and $1/N_c^2$ pure terms that increase the error for small number of simulators, unlike DSMC94, for which the $1/N_c$ term has a negative sign.

CONCLUSIONS

A sophisticated DSMC method recently proposed by the originator of the DSMC method has been implemented, and its accuracy and convergence have been studied. The proposed changes in DSMC include a nearest-neighbor collision-partner selection scheme and a variable adaptive local time-step approach. Collisions are distributed over the duration of a time step and are no longer calculated at the end of the global time step.

The sophisticated method offers significant performance enhancements without any degradation of accuracy. Situations that have solutions of the Boltzmann equation in the continuum, near-continuum, and non-equilibrium regimes are studied. The sophisticated DSMC method is found to be in excellent agreement with these solutions.

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