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Convergence behavior of a new DSMC algorithm

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ABSTRACT

The convergence rate of a new direct simulation Monte Carlo (DSMC) method, termed "sophisticated DSMC", is investigated for one-dimensional Fourier flow. An argon-like hard-sphere gas at 273.15 K and 266.644 Pa is confined between two parallel, fully accommodating walls 1 mm apart that have unequal temperatures. The simulations are performed using a one-dimensional implementation of the sophisticated DSMC algorithm. In harmony with previous work, the primary convergence metric studied is the ratio of the DSMC-calculated thermal conductivity to its corresponding infinite-approximation Chapman–Enskog theoretical value. As discretization errors are reduced, the sophisticated DSMC algorithm is shown to approach the theoretical values to high precision. The convergence behavior of sophisticated DSMC is compared to that of original DSMC. The convergence of the new algorithm in a three-dimensional implementation is also characterized. Implementations using transient adaptive sub-cells and virtual sub-cells are compared. The new algorithm is shown to significantly reduce the computational resources required for a DSMC simulation to achieve a particular level of accuracy, thus improving the efficiency of the method by a factor of 2.

1. Introduction

The direct simulation Monte Carlo (DSMC) method of Bird [1] is the most general and widely used method for simulating non-continuum gas dynamics. DSMC simulations have been shown to yield solutions to the Boltzmann equation in the limit of vanishing discretization error [2–4], and departures of DSMC simulations from such solutions have been shown to obey Green-Kubo theory for small but finite discretization errors [5–7]. As a result, DSMC is often used as the standard by which other methods for simulating non-continuum gas dynamics are assessed.

The generality and the accuracy of the DSMC method have allowed its application to areas outside the regime of hypersonic aerodynamics, such as material processing and micro- and nano-technology. These new areas have placed new demands on the method since the signal-to-noise ratio for subsonic flows is less favorable than for hypersonic flows. Consequently, a clear understanding of how to achieve a specified level of numerical accuracy with a minimum of computational effort is needed.

In response to this need, convergence studies of the DSMC method have been conducted [5–8]. These studies cover a wide range of flows, with the focus on one-dimensional Fourier and Couette flows, both steady and unsteady. The key convergence metric is the ratio of the DSMC-calculated bulk transport properties (thermal conductivity and viscosity) to their Chapman–Enskog (CE) theoretical values [3] although other functionals, such as heat flux and temperature have also been discussed [8].

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Four parameters are known to limit the numerical accuracy of the DSMC method: the number of independent samples per cell S_c, which is related to the statistical error of the method, and the number of simulators (computational molecules) per cell N_c, the time step Δt, and the cell size Δx, which are related to the discretization error of the method [6–8]. Bird observes that statistical fluctuations decrease with the inverse square root of the sample size and can be reduced (in principle) to any desired level by continuing the simulation or by repeating it with different initial random seeds [1]. Several authors [9,10] offer closed-form expressions that relate statistical error in DSMC simulations to the square root of the sample size.

Bird recently proposed a new variant of DSMC, termed "sophisticated DSMC" [11–13]. This new DSMC algorithm aims at improving the computational efficiency of DSMC without losing the accuracy of the original algorithm by reducing the discretization error of the algorithm for a particular selection of simulation parameters. To achieve this, significant modifications to the ways that simulators 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 optimize critical simulation parameters at a relatively low cost, leading to a more efficient DSMC algorithm.

The new method retains many of the features of the original method and all of the physical models. However, the dependence on discretization parameters and therefore the convergence characteristics of the new and original algorithms differ, so a reevaluation of the convergence behavior is therefore necessary.

In this paper, the ability of the new DSMC algorithm to deliver improved computational efficiency is examined. In harmony with previous work [8], the benchmark case used for this purpose is one-dimensional heat transfer in a gas between two parallel walls at unequal temperatures. The main convergence metric used is the ratio of the DSMC-calculated thermal conductivity to its corresponding infinite-approximation CE theoretical value [3]. To ensure that the CE limit is achieved, DSMC simulations are performed at small system and local Knudsen numbers ($\sim$0.02). Under these conditions, the normal solution in the central region of the domain can be clearly differentiated from the Knudsen layers near the walls; it is within this central (near-continuum) region that the convergence behaviors of the functionals are investigated.

More than 700 simulations covering the regime from near-equilibrium to non-equilibrium conditions are performed. The results of the new DSMC method are compared with those of the original method for the same problem. From these results, the difference in the performance of the two algorithms is estimated. The present calculations employ sufficient samples to reduce statistical errors to levels that are negligible compared to the errors associated with the other three parameters. The remaining non-statistical error (hereafter referred to as the discretization error) is systematically investigated for the Fourier problem over wide ranges of the discretization parameters Δx, Δt, and N_c. Herein, DSMC07 and DSMC94 (i.e., as published in Bird's 1994 monograph [1]) are used to distinguish the new and original DSMC algorithms.

2. DSMC07: A new DSMC algorithm

The sophisticated DSMC07 algorithm retains the basic elements of the original DSMC94 algorithm described in Bird's monograph [1]. The key computational assumptions of DSMC, the uncoupling of molecular motion and collisions over a computational time step (usually a fraction of the mean collision time (MCT) or the mean transit time (MTT)) and the partitioning of the physical domain into cells (usually a fraction of the local mean free path), are maintained. The major modifications to the algorithm involve changing how simulators are selected for collisions and how collisions are distributed over the duration of a time step. Besides the global time that a DSMC algorithm keeps track of, simulator-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 the DSMC94 algorithm. Unlike the DSMC94 algorithm, only a small fraction of the simulators move and collide at any global time step.

2.1. Collision partner selection procedures

In DSMC, the computational grid serves two purposes. The first one is the spatial discretization of sampled properties, such as the collision frequency and moments of the molecular velocity distribution (e.g., density, momentum, energy). The second one is to facilitate selection of collision partners that satisfy the basic requirement of geometrical proximity. In principle, computational cells are not necessary for the selection of collision partners. Simulators occupy positions in physical three-dimensional space, and, when collisions between them occur, each simulator could assess its neighboring simulators to identify possible collision partners. Computationally, such a scheme would be feasible only for one-dimensional flows where simulators could be easily sorted using their x-distance. In two- and three-dimensional flows, sorting simulators according to their distances is more complicated, so cells are used to limit the number of possible collision partners while at the same time ensuring geometrical proximity.

This basic principle is what DSMC07 aims to exploit by replacing the random selection of collision partners with a deterministic nearest-neighbor selection scheme, resulting in a smaller mean collision separation (MCS) between colliding simulators [11,12]. The nearest-neighbor selection is limited to the simulators within each cell.

The idea of performing an $O(N^2)$ operation to sort all N simulators in a cell was initially demonstrated by LeBeau et al. [14] and is termed the virtual sub-cell (VSC) scheme. The VSC scheme actually provides an efficient way of performing collisions