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Convergence analysis of the direct simulation Monte Carlo based on the physical laws of conservation

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ABSTRACT

Computational errors in the direct simulation Monte Carlo method can be categorized into four types; decomposition (or discretization), statistical, machine, and boundary condition errors. They arise due to variety of reasons including decoupling of movement and collision phases into two separate steps, finiteness of molecule numbers and domain cell-size, existence of statistical fluctuations and uncertainty, using machines to solve physical problems numerically, computational implementation of boundary conditions of approximate nature, and, finally, assumptions and simplifications adopted in the inter-molecular collision models. In this study, a verification method based on the physical laws of conservation, which are an exact consequence of the Boltzmann equation, is introduced in order to quantify the errors of the DSMC method. A convergence history according to the new verification method is then presented that can illustrate the effects of all type of errors during the simulation run. Convergence analysis indicates that the DSMC method can satisfy the conservation laws with an acceptable level of precision for the flow problems studied. Finally, it is shown that the overall deviation from conservation laws increases with decreasing sample size value and number of particles, and with increasing length of cells and time-step interval size.

1. Introduction

The kinetic Boltzmann equation is considered the foundation for theoretical studies of rarefied gas flows. However, solving the Boltzmann equation directly in phase space is not an easy task because of the complexity and non-linearity of the collisional term [1]. For this reason, analytical study of the equation has been limited to simple flows. As an alternative, the direct simulation Monte Carlo (DSMC) was introduced by Bird to simulate directly the molecular behavior of non-equilibrium gas flows [2–4]. In the DSMC method, a large number of particles are represented by one simulated particle so that the cost of the DSMC method is considerably lower than the molecular dynamics simulation of particles. Owing to its computational simplicity and accuracy, the DSMC method is now being used in various applications: not only for traditional rarefied hypersonic gas flows, but also for micro-scale gases, material processing, acoustic agglomeration processes, and gaseous mixing [5–10].

Generally, computational errors in the DSMC method can be categorized into four types; decomposition (or discretization), statistical, machine, and boundary condition errors. The four types of error and associated computational parameters are depicted in Fig. 1. The decomposition error arises from decoupling of the motion and collision phases into two segregated steps in the DSMC method. The statistical error is generated due to the statistical nature of the DSMC method. The machine error, so-called 'round-off-error,' is inevitable in any numerical method. However, the machine error can easily be minimized using 64-bit data type variables [11].

In the past, much effort has been devoted to the analysis of decomposition and statistical errors in order to enhance the accuracy of the DSMC method. The decomposition error—the most important type—is basically a function of three computational parameters: time-step (Δt), cell-size (Δx), and the number of particles (N) [3]. As Wagner [12] proved theoretically, the DSMC solution will converge to the solution of Boltzmann equation of *a gas undergoing binary collisions between gas particles*, if the value of these parameters are chosen properly (and when no wall surface boundary condition is involved in the simulation). In passing it must be noted that the Boltzmann theory has not been fully worked out for modifying the collision term that should correctly reflect *the molecular collision with the wall surface atoms*. This—subtle, but often neglected—point has already been noticed by various previous studies like Cercignani [13] and Villani [14], in

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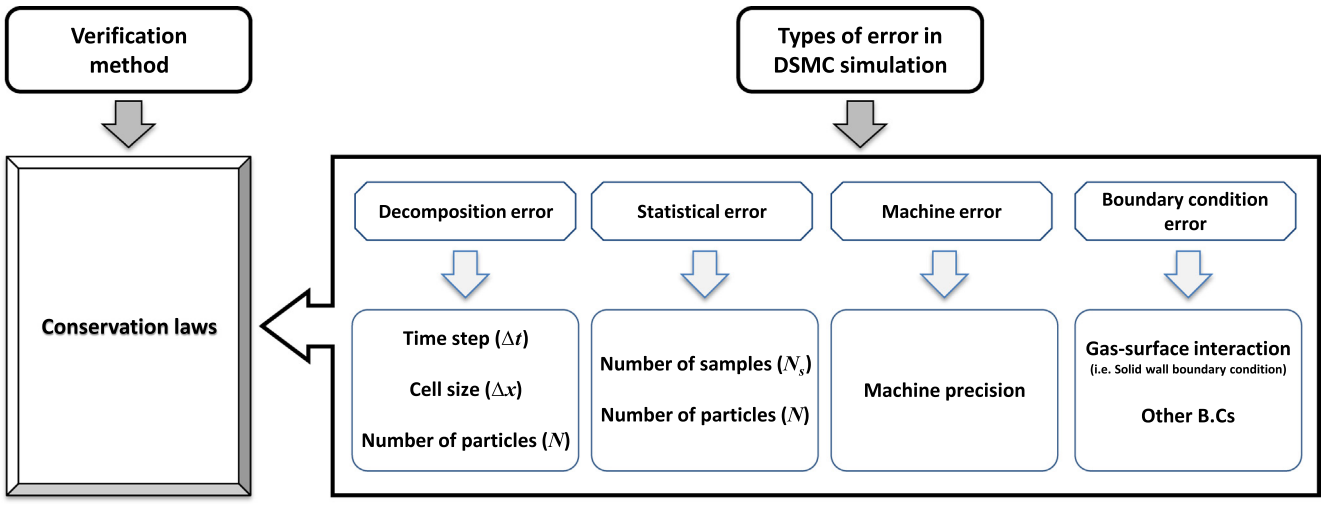

Fig. 1. Types of errors in the DSMC simulation.

which it was stated: "*These conservation laws should hold true when there are no boundaries. In presence of boundaries, conservation laws may be violated: momentum is not preserved by specular reflection, neither is energy if the gas is in interaction with a wall kept at a fixed temperature.*" Thus, the DSMC solution of gaseous flow problems (with no wall surface boundary conditions) can be considered a statistical solution of the Boltzmann equation when infinite numbers of particles are used, and when the values of time-step and cell-size approach zero. Nevertheless, the values of time-step and cell-size cannot be taken as infinitesimally small in reality, due to limitation of numerical computation. Consequently, the decomposition error will always exist and influence the accuracy of the DSMC method. Bird [3] presented two conditions that the time-step value must be a fraction of the mean collision time and the cell-size value should be smaller than the mean free path. He also suggested that the number of particles per cell should be greater than 20. Later, Meiburg [15] showed that these parameters need to be examined more carefully in order to yield accurate results.

Many studies have been also conducted to investigate the effects of computational parameters on decomposition error, and to quantify the amount of error associated with them. For example, Alexander et al. [16] studied a one-dimensional stationary problem, in the limit of infinite number of particles and vanishing time-step value, in order to analyze the role of cell-size on decomposition error. They found that the error comes from the collision pair selection division where particle partners are selected from any place throughout the collision cell. Hadjiconstantinou [17] derived an explicit expression for describing the influence of time-step value on the decomposition error. Garcia and Wagner [18] compared the measured transport coefficients by DSMC with the results obtained from the Green–Kubo theory. They found that the time-step error is closely connected to re-collision phenomena. Rader et al. [19] compared the value of bulk thermal conductivity calculated by the DSMC simulation with results of the Chapman–Enskog theory. The difference between the DSMC and the theoretical result was found less than 0.2% at a given fine value of computational parameters. Interestingly, they also reported that the convergence behavior of error becomes much more complicated when all three parameters are considered simultaneously. Rader et al. [11] also studied the convergence behavior as function of temperature and heat flux in various configurations of the DSMC algorithms. They found that the computational parameters can affect the accuracy of the high order moment properties (e.g., heat flux), more than the first order moment, conserved, properties (e.g., temperature).

The DSMC method utilizes stochastic numerical procedures; hence, it inherits the statistical features of probabilistic methods such as random fluctuation and statistical uncertainty. Moreover, the probability sampling process is added to filter out statistical uncertainty and to estimate the mean value of the estimators. The statistical error can be, in general, reduced by increasing the sample size. However, the statistical uncertainty will not vanish completely because of the finite sample size in the DSMC process. The sample size is basically a function of number of particles and sample steps. Therefore, the magnitude of statistical error is inversely proportional to the square root of the number of particles and the sample steps [3,20].

Recently, there have been several studies on the analysis of statistical error in the DSMC method. Mansour et al. [21] estimated the amount of statistical error for temperature variable by considering hydrodynamic fluctuations in dilute gas. Chen and Boyd [20] analyzed the effect of the number of particles, and the number of sample steps on the statistical error. Hadjiconstantinou et al. [22] also studied the behavior of statistical fluctuations utilizing equilibrium statistical mechanics. They derived a mathematical expression of statistical error for hydrodynamic variables in order to predict the required number of sample steps.

In all previous studies, however, just one type of error (i.e., either decomposition or statistical error) was considered in the analysis while other types of error were neglected by assuming given values for relevant parameters. Moreover, only limited quantities (e.g., transport coefficients and temperature) in simple situations were considered, even though all hydrodynamic variables (e.g., density, velocity, shear stress) are required for full understanding of the behavior of errors. In the present work, in order to overcome these shortcomings, a new verification method based on the exact physical laws of conservation—mass, linear momentum, and total energy—is introduced. *To the best knowledge of the authors, no verification method and consequent convergence analysis of DSMC based on the physical laws of conservation have been reported in the literature.* It must be reiterated that the physical laws of conservation is an *exact* consequence of the Boltzmann equation owing to the property of collisional invariances of mass, momentum, and total energy. Therefore, all the computational methods intended to solve the Boltzmann equation accurately must satisfy in principle the laws of conservation as well.