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An analysis of the convergence of the direct simulation Monte Carlo method

Cyril Galitzine *, Iain D. Boyd

University of Michigan, Department of Aerospace Engineering, Ann Arbor, MI 48109, United States

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ABSTRACT

In this article, a rigorous framework for the analysis of the convergence of the direct simulation Monte Carlo (DSMC) method is presented. It is applied to the simulation of two test cases: an axisymmetric jet at a Knudsen number of 0.01 and Mach number of 1 and a two-dimensional cylinder flow at a Knudsen of 0.05 and Mach 10. The rate of convergence of sampled quantities is found to be well predicted by an extended form of the Central Limit Theorem that takes into account the correlation of samples but requires the calculation of correlation spectra. A simplified analytical model that does not require correlation spectra is then constructed to model the effect of sample correlation. It is then used to obtain an a priori estimate of the convergence error.

1. Introduction

Error in Monte Carlo particle methods, such as e.g. DSMC (direct simulation Monte Carlo), can be defined, in the broadest possible sense, as the difference between the statistical properties of the computational particles and the corresponding moments of the exact solution of the equation being discretized. This error originates from multiple sources which either mitigate or reinforce one another. The first type of error is that introduced by the use of a finite number of samples k to estimate the statistical properties of the particles in the simulation. It will be referred to as the *convergence error* in this article. Error can also come from the use of finite numerical parameters in the application of the particle method which introduces error due to the numerical scaling (as each computational particle represents W_p physical particles, and both time and space are discretized). This error is most commonly due to the use of a too small number of particles N_p, a too large time step Δt, or too large cells. This type of error will be termed *numerical error* in the following. Error can also be due to the inability of the method, in the absence of numerical error, to reproduce the moments of the PDE being discretized. This issue will not be addressed in the present work noting that DSMC, the method used in this article, has been shown to consistently model the homogeneous Boltzmann equation [1] in the limit of $N_p \to \infty$.

Convergence error, the focus of this article, is referred to as the statistical error in [2] and was found in [3] to vary as $A\,(N \times k)^{-1/2}$. The same result was later obtained in [4]. The error was related in [2] to the physical fluctuations in the gas and closed form expressions were obtained in terms of non-dimensional flow numbers for A. From an error perspective, the role of sampling in a DSMC simulation is to reduce the convergence error affecting the quantities being sampled for. Despite the previous investigations of the convergence error cited above, there are no clear requirements within the DSMC community as to the number of sampling steps required to obtain accurate or converged results for those sampled

* Corresponding author.
E-mail address: cyrilg@umich.edu (C. Galitzine).

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properties. Often an arbitrarily large number of samples, e.g. 10^5 [5] is used without further considerations or the sampling period is extended [6] "until the statistical error is small enough". This situation is, in no small part, due to the correlation between samples which prevents the use of the Central Limit Theorem [7]. For instance, the predictions for the statistical error due to finite sampling presented in [2] only hold in the absence of correlation between samples which leads its authors to sample only every 250 time steps in the DSMC simulations conducted to validate them. Many authors also try to reduce the correlation between successive samples by only sampling every few time steps such as [8] or [9] to obtain more independent samples. This shows that the time correlation between samples in DSMC simulations is a well known issue although it has not been accounted for in any existing work about the convergence error. The present article thus aims to derive expressions for the convergence error that take the correlation of samples into account.

The objective of this article is furthermore to present an investigation of the convergence error within the framework of a test case that is sufficiently complex so as to highlight features or phenomena that users of the method are likely to encounter in practice. To accomplish this, instead of using a relatively simple canonical test case such as channel flow [10,2,11], two more complex cases are investigated. The first consist of an axisymmetric supersonic jet, which is a configuration of great practical interest to the rarefied gas dynamics community [12]. The second test case is a two-dimensional hypersonic cylinder flow which is often used for numerical studies [13,14].

In this paper, a rigorous formal definition of the convergence error in Monte Carlo particle simulations is first presented. The goal of the article is to provide an expression for the value of the convergence error that can be used for its a priori determination during the course of the simulation. As previously mentioned, the convergence error is greatly affected by the time correlation between samples. This makes it necessary to quantify the correlation between samples, an issue which is discussed in Section 3. A Central Limit Theorem that takes correlation into account is then introduced. It provides an expression for the aforedefined convergence error in terms of the autocorrelation function of samples. This expression can readily be used "on the fly" during the simulation to assess the convergence of cellwise sampled quantities. Convergence error predictions are then assessed within the framework of the two previously mentioned test cases.

2. Framework for error analysis

2.1. Implementation of the DSMC procedure

A simple argon gas in a two-dimensional (or axisymmetric) domain $\Omega = \{(x, y)\} \subset \mathbb{R}^2$ with velocities in $\mathbb{R}^3$ is considered. $\overline{\Omega}$ is decomposed into N_c quadrangular cells $\{\Omega_i\}_{i=1}^{N_c}$ of respective volume $\{V_i\}_{i=1}^{N_c}$ via quadrangulation Ω_h:

$$\overline{\Omega} = \bigcup_{\Omega_i \in \Omega_h} \Omega_i \tag{1}$$

such that $\mathrm{V}_i \leq h,\ \forall\ 1 \leq i \leq N_c$. The number density n_i in cell i that contains N_i particles is obtained with

$$n_i = \frac{W_p N_i}{V_i}, \tag{2}$$

each computational particle representing W_p physical particles so that the entire domain contains N_p particles. A constant time step Δt and scaling factor W_p are used throughout the domain. The axisymmetric move procedure detailed in [15] p. 371 is employed for the first test case while a standard Euler explicit scheme is used for the second which is two-dimensional. The standard NTC (No Time Counter) collision scheme [15] is used to calculate the number of potential collisions in each cell:

$$N_{\mathrm{coll},i} = \frac{1}{2\mathrm{V}_i} W_p \Delta t N_i \overline{N}_i \left(\sigma g\right)_{\max,i}, \tag{3}$$

where $\overline{N}_i$, the average number of particles in the cell, is obtained by an exponential moving average with a relaxation factor of 0.001. Binary elastic collisions are modeled via the variable hard sphere model [15] with a reference diameter of 4.17×10^{-10} m at 273 K and a temperature exponent of 0.81. Further details concerning our implementation of the DSMC procedure can be found in [16].

2.2. Cell and particle based variables

Any variable characterizing particle j at time t^k is denoted by $\mathbf{y}_j^k$ with $1 \leq j \leq N_p$ which can for instance represent its instantaneous position $\vec{\mathbf{x}}_j^k$ or velocity $\vec{\mathbf{v}}_j^k$. Cell-based quantities are denoted by y_i^k with $1 \leq i \leq N_c$ which designates any variable specific to cell i at time t^k such as the number of particles contained in the cell N_i^k. When all particles or all cells of the simulations are simultaneously considered, particle and cell-based quantities can both be represented by a series of vectors, namely $\vec{\mathbf{y}}^k = \left(\mathbf{y}_1^k, \ldots, \mathbf{y}_{N_p}^k\right)$ and $\vec{y}^k = \left(y_1^k, \ldots, y_{N_c}^k\right)$. The average value of $\mathbf{y}$ in cell Ω_i at time step k is naturally defined as: