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Convergence of A Distributional Monte Carlo Method for the Boltzmann Equation

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Abstract. Direct Simulation Monte Carlo (DSMC) methods for the Boltzmann equation employ a point measure approximation to the distribution function, as simulated particles may possess only a single velocity. This representation limits the method to converge only weakly to the solution of the Boltzmann equation. Utilizing kernel density estimation we have developed a stochastic Boltzmann solver which possesses strong convergence for bounded and L^∞ solutions of the Boltzmann equation. This is facilitated by distributing the velocity of each simulated particle instead of using the point measure approximation inherent to DSMC. We propose that the development of a distributional method which incorporates distributed velocities in collision selection and modeling should improve convergence and potentially result in a substantial reduction of the variance in comparison to DSMC methods. Toward this end, we also report initial findings of modeling collisions distributionally using the Bhatnagar-Gross-Krook collision operator.

AMS subject classifications: 82B40, 76P05, 65C35, 82C80

Key words: Direct simulation monte carlo, rarefied gas dynamics, Boltzmann equation, convergence proof.

1 Introduction

Direct Simulation Monte Carlo (DSMC) is a stochastic simulation method which approximates the physics of the Boltzmann equation on a set of simulated particles. The method was originally developed in the mid-1960's by Bird [8, 9], and is based on a probabilistic simulation of the motions and interactions of a fraction of the total number of particles in the gas. The method relies on an approximation known as the uncoupling principle, which allows intermolecular collisions to be decoupled from particle convection [17].

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Initially, the DSMC method was met with some trepidation. Although remaining true to the principles of kinetic theory, the method itself was not formally derived from the Boltzmann equation, the governing equation of kinetic theory. In its simplest form, the Boltzmann equation describes the evolution of the molecular velocity probability density function, $f : (\mathbb{R}^3 \times \Lambda \times \mathbb{R}) \to \mathbb{R}^+$. The function is defined over a seven dimensional space which includes three dimensions of velocity components, three dimensions of physical space in the domain $\Lambda \subseteq \mathbb{R}^3$, and the additional dimension of time. The term velocity distribution function is used under various definitions in the literature, all of which represent some scaled form of the probability density function for molecular velocity. Throughout this paper the term velocity distribution function taken to mean the probability density function for molecular velocity and will be denoted by f.

The Boltzmann equation accounts for changes to f due to three influences: particle convection, acceleration of particles by external forces, and intermolecular collisions. The equation may be modified to include the distribution of energy over various internal energy modes, but for simplicity we consider only the basic case of a simple, monatomic gas. In this case, the Boltzmann equation is given by

$$\frac{\partial}{\partial t} f(\vec{r},\vec{c},t) + \vec{c} \cdot \frac{\partial}{\partial \vec{r}} f(\vec{r},\vec{c},t) + \vec{F} \cdot \frac{\partial}{\partial \vec{c}} f(\vec{r},\vec{c},t) = J[f](\vec{r},\vec{c},t).$$

Here $\vec{r}$ is the spatial variable, $\vec{c}$ is the velocity variable, t is the temporal variable, and $\vec{F}$ is any externally applied forcing. The collision integral J is defined as

$$\begin{aligned}[f](\vec{r},\vec{c},t) = \int_{R^3} \int_{S_2^+} \big[& f(\vec{r},\vec{c'}(\vec{c},\vec{c_1},\vec{\Omega}),t) f(\vec{r},\vec{c_1'}(\vec{c},\vec{c_1},\vec{\Omega}),t) \\ & - f(\vec{r},\vec{c},t) f(\vec{r},\vec{c_1},t) \big] g\sigma(g,\Omega) d\vec{\Omega} d\vec{c_1},\end{aligned}$$

where S_2^+ denotes the positive half of the unit sphere in $\mathbb{R}^3$, $\vec{\Omega}$ is the collision orientation vector, σ is the collision cross section, $g = \|\vec{c} - \vec{c_1}\|$, and $\{\vec{c'}, \vec{c_1'}\}$ are the post-collision velocities given by

$$\vec{c'}(\vec{c},\vec{c_1},\vec{\Omega}) = \frac{1}{2}\big[(\vec{c_1} + \vec{c}) - g\vec{\Omega}\big], \tag{1.1a}$$

$$\vec{c_1'}(\vec{c},\vec{c_1},\vec{\Omega}) = \frac{1}{2}\big[(\vec{c_1} + \vec{c}) + g\vec{\Omega}\big]. \tag{1.1b}$$

In 1980, Nanbu [17] proposed the first DSMC method derived directly from the Boltzmann equation, and in 1989, Babovsky and Illner proved weak convergence of Nanbu's method for L^1 solutions of the space-homogeneous [5], and space-inhomogeneous [6], Boltzmann equations. Wagner [22] established similar convergence for Bird's method in 1992, giving DSMC a firm theoretical foundation.

The DSMC method also has inherent drawbacks. A significant number of particles must be simulated to achieve realistic results. This raises storage issues as the position