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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.

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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

and velocity vectors of each simulated particle must be stored throughout the simulation. Selection of representative collisions over these potentially large data arrays introduces a non-trivial burden on the simulation process. Furthermore, the stochastic nature of the simulation introduces a significant amount of variation in the results and consequently, data must be averaged over an ensemble to improve the quality of the solution. This variance is significantly troublesome in the case of low Mach number rarefied flows [1].

Despite these drawbacks, DSMC has gained general acceptance in the field of rarefied gas dynamics and is the standard computational method employed when increased accuracy over the continuum equation sets (Euler, Navier-Stokes, etc.) is required. Although other methods for approximating solutions to the Boltzmann equation exist (e.g., see [4,13,16,18,19]), they are either plagued by increased computational demands or are not fully consistent with the physics described by the Boltzmann equation. Consequently, development of improved DSMC algorithms remains an area of active research. Recently significant progress has been achieved in the development of variance reduced DSMC schemes for low signal flows (see [1–3, 14]). Monte Carlo schemes which employ particle simulation to model only the deviation from thermodynamic equilibrium have also been developed (see [14, 23]). These developments have improved the practicability of DSMC by attempting to combat the aforementioned drawbacks.

We observe that existing convergence theorems for DSMC methods are fairly weak, and amount to convergence in moments of the distribution function for well-behaved test functions (bounded, continuous). In fact, DSMC does not directly solve the Boltzmann equation for the distribution function, but rather simulates the physics of the Boltzmann equation on the collection of simulated particles. One of the major limitations to stronger forms of convergence is the singular nature of the simulated particle velocities. Specifically, since one simulates only a fraction of the number of actual particles, each simulated particle represents $W = N/N_p$ actual particles, where N is the total number of particles and N_p is the number of simulated particles. In practice W may be on the order of 10^6 or more. As a simulated particle can possess only a single velocity vector, the simulation must approximate the distribution function in terms of point measures. Therefore, when considering the overall distribution function in the gas, we obtain

$$\hat{f}(\vec{c}) = \frac{1}{N_p}\sum_{i}^{N_p}\delta(\vec{c}-\vec{c}_i), \tag{1.2}$$

where $\vec{c}_i$ is the velocity vector of the i^{th} particle. A convergent DSMC algorithm can therefore only achieve convergence in probability measure. Namely

$$\langle \phi, \hat{f}\rangle \to \langle \phi, f\rangle,$$

for any bounded, continuous ϕ on $\mathbb{R}^3$.

To illustrate the weakness of this the convergence associated with this approximation, consider the cumulative error between an approximate solution and any

bounded solution of the Boltzmann equation which we define as

$$e(\hat{f}) = \int_{\mathbb{R}^3} |\hat{f}(\vec{c},t) - f(\vec{c},t)| d\vec{c}. \tag{1.3}$$

Let $M(t)$ denote the subset of $\mathbb{R}^3$ on which $\hat{f}$ takes on a nonzero value. Clearly, $M(t)$ is a set of measure zero. Note also that

$$\int f(\vec{c}) d\vec{c} = 1,$$

as f is a probability density function. Then if the Boltzmann equation has a bounded solution f, the cumulative error of the Nanbu approximation to f is given by

$$\begin{aligned} e(\hat{f}) &= \int_{\mathbb{R}^3} |\hat{f}(\vec{c},t) - f(\vec{c},t)| d\vec{c} \\ &= \int_{\mathbb{R}^3 - M(t)} |\hat{f}(\vec{c},t) - f(\vec{c},t)| d\vec{c} + \int_{M(t)} |\hat{f}(\vec{c},t) - f(\vec{c},t)| d\vec{c} \\ &= \int_{\mathbb{R}^3 - M(t)} |f(\vec{c},t)| d\vec{c} = 1. \end{aligned}$$

This demonstrates that not only does Nanbu's method fail to converge in this sense, but the cumulative error is independent of the number of simulated particles and the time step. As each particle represents W actual particles, the representation of a velocity distribution by a sum of delta functions is nonphysical whenever $N_p < N$. The probability that any two particles share the exact velocity is zero. Furthermore, as observed by Rjasanow and Wagner [20] each simulated particle represents a large ensemble of actual particles and therefore it is natural that a collision causes velocity changes only for a portion of that ensemble. We suggest that a method which forgoes the point measure representation of the distribution function in favor of a more realistic approximation will achieve improved convergence results. Toward this end, we have begun development of "Distributional Monte Carlo" (DMC) methods. In DMC, replace the point measure representation of the distribution function by allowing each simulated particle to possess a nonsingular velocity distribution function.

In Section 2, we begin with a brief discussion of kernel density estimation which we utilize to approximate the velocity distribution function. Section 3 contains a detailed discussion and mathematical justification of the method we propose. We prove weak convergence for L^1 solutions of the space homogeneous Boltzmann equation, strong convergence for solutions which are L^∞, and pointwise convergence for bounded solutions. To our best knowledge, no existing DSMC schemes have been formally proven to exhibit these forms of convergence. Section 3 concludes with a numerical example of the implementation of this scheme. Section 4 presents some initial steps towards the development of a fully distributional method, and we summarize our major findings in Section 5.

2 Kernel density estimation

Kernel Density Estimation (KDE) is a technique for estimating the probability density function of a random variable $X \in \mathbb{R}^d$ from a set of discrete samples as follows [24]

$$\hat{f}(x;h) = \frac{1}{Nh^d} \sum_{i=1}^{N} K\Big(\frac{x - X_i}{h}\Big). \tag{2.1}$$

Here, N is the number of discrete samples, X_i the value of the i^{th} sample, $h \in \mathbb{R}^+$ the kernel bandwidth and $K \in L^2$ the kernel function. The kernel function must satisfy the following conditions

$$\int K(x)dx = 1, \tag{2.2a}$$

$$\int xK(x)dx = 0. \tag{2.2b}$$

The problem then becomes one of determining a suitable K and h with which to approximate the distribution function. The value of h is chosen to minimize the error between the estimator and the actual distribution function in some sense. If h is too small, the estimator will exhibit overly oscillatory behavior. It h is too large, subtle features of the distribution function may not be captured by the estimator. Wand [24] shows that the asymptotic mean square error between f and $\hat{f}$ is minimized when

$$h = \Big[\frac{m(K)}{(\mu_2(K))^2 m(f'')N}\Big]^{\frac{1}{5}}, \tag{2.3}$$

where

$$m(g) = \int [g(x)]^2 dx, \qquad \mu_2(g) = \int x^2 g(x)dx.$$

Notice that calculation of such an h requires not only that f'' is known, but also that $f \in W^{2,2}$. If f is normal with variance σ^2, Eq. (2.3) becomes,

$$h = \Big[\frac{8\sqrt{\pi}m(K)}{3(\mu_2(K))^2 N}\Big]^{\frac{1}{5}}\sigma. \tag{2.4}$$

3 DMC-KDE

Observe that the Nanbu approximation to the distribution function may be viewed as a special case of a kernel density estimator with $K = \delta$ and $h = 1$. Recognizing this similarity, we developed a distributional Monte Carlo method employing some of the results from kernel density estimation. We have termed this approach DMC-KDE. It should be noted that KDE has been applied in the Variance Reduced DSMC (VRDSMC) approach proposed by Al-Mohssen and Hadjiconstantinou [1–3] though in that application it was employed only as a smoothing and stabilization technique.

In this section, we discuss the mathematical details of the new method, prove weak convergence for L^1 solutions of the space homogeneous Boltzmann equation, as well as strong convergence for L^∞ solutions and pointwise convergence for bounded solutions. We then present results of a numerical implementation of the method.

3.1 Derivation and mathematical justification

In the Distributional Monte Carlo approach we allow each simulated particle to possess its own velocity distribution function, f_i. The overall distribution function in the gas is then given by

$$f = \frac{1}{N}\sum_{i=1}^{N_p} f_i. \tag{3.1}$$

In the DMC-KDE approach, we make the simplification that each particle's velocity is distributed according to a prescribed distribution, that is

$$f_i(\vec{c}) = \frac{1}{h^3}\sum_{i=1}^{N_p} K\Big(\frac{\vec{c}-\vec{c}_i}{h}\Big). \tag{3.2}$$

The mean of each particle's distribution function $\vec{c}_i$ is allowed to vary, but the kernel function and bandwidth are chosen to be identical for all particles. Therefore the approximation to the overall distribution function of the gas is given by

$$\tilde{f}(\vec{c};h) = \frac{1}{N_p h^3}\sum_{i=1}^{N_p} K\Big(\frac{\vec{c}-\vec{c}_i}{h}\Big). \tag{3.3}$$

Choosing

$$h : \mathbb{N} \to \mathbb{R}^+,$$

with the property

$$\lim_{N_p\to\infty} h(N_p) = 0,$$

and K is chosen as described in the previous section, Eq. (3.3) is observed to be a kernel density estimator for f. Although we prove that convergence is guaranteed for any such h and K, it is necessary to choose specific values of such parameters from which to construct a simulation scheme. On the basis of physical reasoning we choose a Gaussian kernel for K and utilize Eq. (2.4) to determine h.

$$K(\vec{x}) = (2\pi)^{-\frac{3}{2}}\exp\Big(-\frac{\|\vec{x}\|^2}{2}\Big), \tag{3.4a}$$

$$h = \Big[\frac{32}{3\sqrt{2}N_p}\Big]^{\frac{1}{5}}\sigma_{est}, \tag{3.4b}$$

where σ_{est} is an estimation of the standard deviation of f. These choices are advantageous for a number of reasons. Since h is chosen such that $h\to 0$ as $N_p\to\infty$, Eq. (3.3)

will converge to the delta representation when N_p becomes large recovering the point measure approximation of DSMC. Further, the distribution function of each simulated particle is Maxwellian, the prevailing distribution in an equilibrium gas. The interpretation therefore is that although the collection of particles that a simulated particle represents all possess different velocities, as a collection the particles are in equilibrium with one another. This represents a relaxation of the assumption made by DSMC that the collection of particles possess the same singular velocity. To develop the mathematical formulation of this approach, we follow an analysis similar to Nanbu [17].

Beginning with Eq. (3.3) we seek to determine the evolution of the distribution function due to intermolecular collisions through the time interval Δt. We begin by utilizing a forward Euler discretization

$$f(\vec{c}, t+\Delta t) = f(\vec{c}, t) + \Delta t \frac{\partial f}{\partial t}(\vec{c}, t), \tag{3.5}$$

where $\partial f/\partial t$ is obtained from the space homogeneous Boltzmann equation

$$\frac{\partial f}{\partial t}(\vec{c}, t) = J[f](\vec{c}, t). \tag{3.6}$$

Substituting Eq. (3.3) into Eq. (3.6), one obtains

$$\frac{\partial f}{\partial t} = \frac{1}{N_p^2} \sum_{i=1}^{N_p} \sum_{j=1}^{N_p} (S_{ij} - T_{ij}), \tag{3.7}$$

where

$$S_{ij} = \frac{1}{h^6} \int_{\mathbb{R}^3} \int_{S_2^+} K\Big(\frac{\vec{c'} - \vec{c}_i}{h}\Big) K\Big(\frac{\vec{c_1'} - \vec{c}_j}{h}\Big) \cdot g\sigma(g, \vec{\Omega}) d\Omega d\vec{c_1}, \tag{3.8a}$$

$$T_{ij} = \frac{1}{h^6} \int_{\mathbb{R}^3} \int_{S_2^+} K\Big(\frac{\vec{c} - \vec{c}_i}{h}\Big) K\Big(\frac{\vec{c_1} - \vec{c}_j}{h}\Big) \cdot g\sigma(g, \vec{\Omega}) d\Omega d\vec{c_1}. \tag{3.8b}$$

Substituting Eqs. (3.4a) and (1.1a)-(1.1b) into Eq. (3.8a), one obtains

$$S_{ij} = \frac{1}{2\pi h^6} \int_{\mathbb{R}^3} G(\vec{c}, \vec{c_1}) \exp\Big\{ -\frac{1}{4h^2} [{c_1}^2 + c^2 + {c_i}^2 + {c_j}^2 - (\vec{c_i} + \vec{c_j}) \cdot (\vec{c_1} + \vec{c})] \Big\} g d\vec{c_1}, \tag{3.9}$$

where

$$G(\vec{c}, \vec{c_1}) = \int_{S_2^+} \exp[\vec{a} \cdot \vec{\Omega}] \sigma(g, \vec{\Omega}), \qquad \vec{a} = \frac{g(\vec{c_j} - \vec{c_i})}{4h^2}.$$

Nanbu [17] shows that G may be approximated for small h by the following

$$G(\vec{c}, \vec{c_1}) = 2\pi\sigma(g, \chi) \frac{e^{\|\vec{a}\|}}{\|\vec{a}\|}.$$

Substituting this expression for G into Eq. (3.9) yields

$$S_{ij} = \frac{2}{g_{ij}} \int_{\mathbb{R}^3} \Big\{ \frac{(2\pi)^{-\frac{3}{2}}}{h^3} \exp\Big[- \frac{(\vec{c} + \vec{c_1} - \vec{c_i} - \vec{c_j})^2}{4h^2} \Big] \Big\} \cdot \Big\{ \frac{1}{\sqrt{2\pi}h} \exp\Big[- \frac{(g - g_{ij})^2}{4h^2} \Big] \Big\} \sigma(g, \chi) d\vec{c_1}, \tag{3.10}$$

where $g_{ij} = \|\vec{c_j} - \vec{c_i}\|$. Next, we consider Eq. (3.5) under the limit as $h \to 0$ with $\partial f / \partial t$ as in Eq. (3.7)

$$f(\vec{c}, t + \Delta t) = f(\vec{c}, t) + \frac{\Delta t}{N_p^2} \sum_{i=1}^{N_p} \sum_{j=1}^{N_p} (S_{ij}^* - T_{ij}^*), \tag{3.11}$$

where

$$S_{ij}^* = \lim_{h \to 0} S_{ij}, \qquad T_{ij}^* = \lim_{h \to 0} T_{ij}.$$

Definition 3.1. *Let $\{g_\alpha\}$ be a family of locally integrable functions on $\mathbb{R}_n$. $\{g_\alpha\}$ is called an* n-dimensional delta family *as $\alpha \to \alpha_0$ if*

$$\lim_{\alpha \to \alpha_0} \int_{\mathbb{R}_n} g_\alpha(x) \phi(x) dx = \phi(0),$$

where ϕ is any bounded continuous function on $\mathbb{R}^n$. We write

$$\lim_{\alpha \to \alpha_0} g_\alpha(x) = \delta(x),$$

in conformance with [21].

It can be shown that each of the bracketed terms under the integrand in Eq. (3.10) is a delta family, the first being three-dimensional, the second one-dimensional. Using Eq. (3.8b) and performing a similar analysis, the terms under the integrand for T_{ij} can also be shown to exhibit this behavior. We therefore conclude

$$S_{ij}^* = \frac{4}{g_{ij}} \delta\Big(\|\vec{c^*}\| - \frac{1}{2} g_{ij} \Big) \sigma(g_{ij}, \chi), \qquad T_{ij}^* = g_{ij} \sigma_T(g_{ij}) \delta(\vec{c} - \vec{c_i}).$$

Substituting these terms into Eq. (3.11), one obtains

$$f(\vec{c}, t + \Delta t) = \frac{1}{N_p} \sum_{i=1}^{N_p} \big[(1 - P_i) \delta(\vec{c} - \vec{c_i}) + Q_i(\vec{c}) \big],$$

where

$$P_i = \frac{\Delta t}{N} \sum_{j=1, j \neq i}^{N} g_{ij} \sigma_T(g_{ij}), \qquad Q_i(\vec{c}) = \frac{4 \Delta t}{N} \sum_{j=1, j \neq i}^{N} \frac{\sigma(g_{ij}, \chi)}{g_{ij}} \delta\Big(\|\vec{c^*}\| - \frac{1}{2} g_{ij} \Big), \tag{3.12a}$$

$$\sigma_T(g_{ij}) = \int_{S_2^+} \sigma(g_{ij}, \vec{\Omega}) d\vec{\Omega}, \quad \vec{c^*} = \vec{c} - \frac{1}{2}(\vec{c_i} - \vec{c_j}), \tag{3.12b}$$

and χ is the angle between $\vec{c}^*$ and $\vec{c}_i - \vec{c}_j$. P_i represents the probability that the i^{th} particle collides in the time interval Δt, while the individual terms

$$P_{ij} = \frac{\Delta t}{N} g_{ij} \sigma_T(g_{ij}),$$

represent the probability that the i^{th} particle collides with the j^{th} particle over Δt. Also, notice that Q_i represents the portion of distribution function describing the effects of collisions over the time interval Δt. Having passed to the limit of large N_p (where the distributions tend towards a delta approximation), we have obtained the same result as Nanbu [17] for the evolution of the distribution function over Δt. Therefore, we may reuse the collision selection and modeling rules developed by Nanbu, but with a new interpretation. Namely, $\vec{c}_i$ now represents the mean velocity of the i^{th} simulated particle. Collision interactions therefore have the effect of shifting the individual Maxwellian distributions to new mean values. The stochastic scheme to evolve f through Δt is therefore given as follows:

- For each particle, calculate P_i. Generate a random number r_1 in the interval $(0,1)$. If $P_i > r_1$, accept the particle for collision.
- Sample a collision partner j from the conditional probability distribution $P^*_{ik} = P_{ik}/P_i$, by sampling a second random number r_2 uniformly from the interval $(0,1)$ and identifying the j which satisfies

$$\sum_{k=1}^{j-1} P^*_{ik} < r_2 < \sum_{k=1}^{j} P^*_{ik}.$$

- Sample the direction of $\vec{c}^*$ based on Eq. (3.12), and compute the post collision velocity of the i^{th} particle.

Like DSMC, the simulation would be evolved many times to generate an ensemble averaged solution so as to reduce statistical fluctuations. Nanbu's scheme has in the past been criticized for not mainintaining strict conservation of energy in each collision but only over the ensemble. Since the current scheme employs a similar sampling procedure for the Maxwellian centers, it will not conserve energy with each collision either. This is not a major concern in demonstraiting the benefits of such an approach, and a number of implementable alternative sampling procedures for collision interactions exist which do conserve energy with each collision.

Although the scheme is in some sense similar to Nanbu, the effect of allowing velocities to be distributed has a significant impact on the mathematical convergence properties of the method. Namely, whereas DSMC can only achieve convergence in probability measure (weak convergence), we prove that the DMC-KDE approach results in convergence in solution (strong convergence) for L^∞ and bounded solutions of the Boltzmann equation. Therefore, rather than a stochastic simulator of the Boltzmann equation, the DMC-KDE approach represents a stochastic solver of the Boltzmann equation.

3.2 Convergence of DMC-KDE

In the following, we prove weak convergence of the DMC-KDE approximation for the space homogeneous Boltzmann Equation. Based upon the results of Babovsky and Illner [5, 6] this is not unreasonable to expect. Although in the above work we have chosen specific functions for h and K, our proof is for the more general case.

Let $\{\vec{c}_i\}_{i=1}^{N_p}$ be the mean velocities of the N_p simulated particles at a given time step derived by the above method. The velocity distribution function (VDF) of the DMC-KDE method is then

$$\tilde{f}(\vec{c}) = \frac{1}{N_p h^3} \sum_{i=1}^{N_p} K\Big(\frac{\vec{c}-\vec{c}_i}{h}\Big),$$

where

$$K \in \Big\{ g \in L^2(\mathbb{R}_3) : g(x) \geq 0 \text{ for } \forall x;\ \int_{\mathbb{R}_3} g(x)dx = 1;\ \int_{\mathbb{R}_3} xg(x)dx = 0 \Big\},$$

and $h : \mathbb{N} \to \mathbb{R}^+$ with $\lim_{N_p\to\infty} h(N_p) = 0$. Define $\{f_h\}$ by

$$f_h(\vec{x}) = \frac{1}{h^3} K\Big(\frac{\vec{x}}{h}\Big).$$

Then, $\tilde{f}$ may be rewritten as,

$$\tilde{f}(\vec{c}) = \frac{1}{N_p} \sum_{i=1}^{N_p} f_h(\vec{c}-\vec{c}_i). \tag{3.13}$$

Lemma 3.1. *$\{f_h\}$ is a delta family as $h \to 0$.*

Proof. (see [21]) Let $\vec{u} = \vec{x}/h$. we have

$$\int_{\mathbb{R}_3} f_h(\vec{x})d\vec{x} = \frac{1}{h^3}\int_{\mathbb{R}_3} K\Big(\frac{\vec{x}}{h}\Big)d\vec{x} = \int_{\mathbb{R}_3} K(\vec{u})d\vec{u} = 1.$$

Also, for any $A > 0$,

$$\lim_{h\to0}\int_{\|\vec{x}\|>A} f_h(\vec{x})d\vec{x} = \lim_{h\to0}\frac{1}{h^3}\int_{\|\vec{x}\|>A} K\Big(\frac{\vec{x}}{h}\Big)d\vec{x} = \lim_{h\to0}\int_{\|\vec{u}\|>\frac{A}{h}} K(\vec{u})d\vec{u} = 0,$$

and

$$\lim_{h\to0}\int_{\|\vec{x}\|<A} f_h(\vec{x})d\vec{x} = \lim_{h\to0}\frac{1}{h^3}\int_{\|\vec{x}\|<A} K\Big(\frac{\vec{x}}{h}\Big)d\vec{x} = \lim_{h\to0}\int_{\|\vec{u}\|<\frac{A}{h}} K(\vec{u})d\vec{u} = 1.$$

Now, let ϕ be any bounded and continuous function on $\mathbb{R}^3$. We have,

$$\begin{aligned}\lim_{h\to0}\int_{\mathbb{R}_3} f_h(\vec{x})\phi(\vec{x})d\vec{x} - \phi(0) &= \lim_{h\to0}\Big[\int_{\mathbb{R}_3} f_h(\vec{x})\phi(\vec{x})d\vec{x} - \phi(0)\int_{\mathbb{R}_3} f_h(\vec{x})d\vec{x}\Big] \\ &= \lim_{h\to0}\int_{\mathbb{R}_3} f_h(\vec{x})[\phi(\vec{x})-\phi(0)]d\vec{x}.\end{aligned}$$

Define $\eta(\vec{x}) = \phi(\vec{x}) - \phi(0)$. Let $\epsilon > 0$ and $B > 0$. We have,

$$\int_{\mathbb{R}_3} f_h(\vec{x})\eta(\vec{x})d\vec{x} = \int_{\|\vec{x}\|<B} f_h(\vec{x})\eta(\vec{x})d\vec{x} + \int_{\|\vec{x}\|>B} f_h(\vec{x})\eta(\vec{x})d\vec{x}.$$

Choose $M > 0$ such that

$$|\eta(\vec{x})| \leq M,$$

for $\forall \vec{x}$. Let

$$p(B) = \max_{\|\vec{x}\|<B} |\eta(\vec{x})|.$$

We have,

$$\begin{aligned}\Big|\int_{\mathbb{R}_3} f_h(\vec{x})\eta(\vec{x})d\vec{x}\Big| \leq& \Big|\int_{\|\vec{x}\|\leq B} f_h(\vec{x})\eta(\vec{x})d\vec{x}\Big| + \Big|\int_{\|\vec{x}\|>B} f_h(\vec{x})\eta(\vec{x})d\vec{x}\Big| \\ \leq& p(B)\Big|\int_{\|\vec{x}\|\leq B} f_h(\vec{x})d\vec{x}\Big| + \Big|\int_{\|\vec{x}\|>B} f_h(\vec{x})d\vec{x}\Big| \\ \leq& p(B) + M\Big|\int_{\|\vec{x}\|>B} f_h(\vec{x})d\vec{x}\Big|.\end{aligned}$$

Since η is continuous and $\eta(0) = 0$, there exists $B \in \mathbb{R}$ such that $p(B) < \epsilon/2$. Also, from above we have that there exists $\alpha > 0$, such that

$$\Big|\int_{\|\vec{x}\|>B} f_h(\vec{x})d\vec{x}\Big| < \frac{\epsilon}{2M},$$

whenever $0 < h < \alpha$. Therefore, for any $\epsilon > 0$, we have shown that there exists α such that

$$\begin{aligned}\Big|\int_{\mathbb{R}_3} f_h(\vec{x})\eta(\vec{x})d\vec{x}\Big| &\leq p(B) + M\Big|\int_{\|\vec{x}\|>B} f_h(\vec{x})d\vec{x}\Big| \\ &< \frac{\epsilon}{2} + M\frac{\epsilon}{2M} = \epsilon,\end{aligned}$$

whenever $0 < h < \alpha$. Therefore,

$$\lim_{h\to 0}\int_{\mathbb{R}_3} f_h(\vec{x})\eta(\vec{x})d\vec{x} = 0.$$

Which implies

$$\lim_{h\to 0}\int_{\mathbb{R}_3} f_h(\vec{x})\phi(\vec{x})d\vec{x} = \phi(0),$$

and hence $\{f_h\}$ is a delta family as $h \to 0$. □

Recall that the parameter h is chosen in the DMC-KDE method such that

$$\lim_{N_p\to\infty} h(N_p) = 0.$$

Then $\{f_{h(N_p)}\}$ is a delta family as $N_p \to \infty$ by Lemma 3.1. We will denote this family by $\{f_{N_p}\}$. We next prove that in the limit as $N_p \to \infty$ the probability measure generated by the DMC-KDE approach is the same as that generated by the Nanbu DSMC method.

Lemma 3.2. *For any bounded and continuous ϕ on $\mathbb{R}^3$,*

$$\lim_{N_p\to\infty}\int_{\mathbb{R}_3}\phi(\vec{c})\tilde{f}(\vec{c})d\vec{c}=\lim_{N_p\to\infty}\int_{\mathbb{R}_3}\phi(\vec{c})\hat{f}(\vec{c})d\vec{c}.$$

Proof. Choose any $\epsilon>0$. Then by Lemma 3.1, for any bounded and continuous ϕ, there exists M such that

$$\Big|\int_{\mathbb{R}_3}\phi(\vec{c})f_{N_p}(\vec{c}-\vec{c}_i)d\vec{c}-\phi(\vec{c}_i)\Big|<\epsilon,$$

for all $N_p>M$. Recalling that the DMC-KDE scheme generates the same values for the Maxwellian centers as the Nanbu method generates for molecular velocities, we have

$$\begin{aligned}\Big|\int_{\mathbb{R}_3}\phi(\vec{c})(\tilde{f}(\vec{c})-\hat{f}(\vec{c}))d\vec{c}\Big|=&\Big|\int_{\mathbb{R}_3}\phi(\vec{c})\frac{1}{N_p}\Big(\sum_{i=1}^{N_p}f_{N_p}(\vec{c}-\vec{c}_i)-\delta(\vec{c}-\vec{c}_i)\Big)d\vec{c}\Big|\\ \le&\frac{1}{N_p}\sum_{i=1}^{N_p}\Big|\int_{\mathbb{R}_3}\phi(\vec{c})(f_{N_p}(\vec{c}-\vec{c}_i)-\delta(\vec{c}-\vec{c}_i))d\vec{c}\Big|\\ <&\frac{1}{N_p}\sum_{i=1}^{N_p}\epsilon=\epsilon,\end{aligned}$$

for all $N_p>M$. □

We will also require the following result proven by Babovsky and Illner.

Theorem 3.1. [Babovsky and Illner [5, 6, 10, 11]]. *If the space homogeneous Boltzmann equation has a non-negative solution $f\in L^1$, then the solution $\hat{f}$ of Nanbu's method converges weakly in L^1 to f such that for any bounded, continuous test function ϕ,*

$$\lim_{\Delta t\to 0}\lim_{N_p\to\infty}\int_{\mathbb{R}_3}\phi(\vec{c})\hat{f}(\vec{c})d\vec{c}=\int_{\mathbb{R}_3}\phi(\vec{c})f(\vec{c})d\vec{c}.$$

Combining this result with Lemma 3.2, we have the following theorem.

Theorem 3.2. *If the space homogeneous Boltzmann equation has a non-negative solution $f\in L^1$, then the solution $\tilde{f}$ of the DMC-KDE method converges weakly in L^1 to f such that for any bounded and continuous test function ϕ on $\mathbb{R}^3$,*

$$\lim_{\Delta t\to 0}\lim_{N_p\to\infty}\int_{\mathbb{R}_3}\phi(\vec{c})\tilde{f}(\vec{c})d\vec{c}=\int_{\mathbb{R}_3}\phi(\vec{c})f(\vec{c})d\vec{c}.$$

Proof. Choose any $\epsilon>0$. Then,

$$\begin{aligned}&\Big|\int_{\mathbb{R}_3}\phi(\vec{c})(\tilde{f}(\vec{c})-f(\vec{c}))d\vec{c}\Big|\\ \le&\Big|\int_{\mathbb{R}_3}\phi(\vec{c})(\tilde{f}(\vec{c})-\hat{f}(\vec{c}))d\vec{c}\Big|+\Big|\int_{\mathbb{R}_3}\phi(\vec{c})(\hat{f}(\vec{c})-f(\vec{c}))d\vec{c}\Big|.\end{aligned}$$

Applying Lemma 3.2 and Theorem 3.1 to the terms to the right of the inequality yields the desired result. □

We have therefore proven that the DMC-KDE method exhibits the same convergence as Nanbu's method in the general case, namely convergence in probability measure. We next prove that stronger forms of convergence are possible compared with Nanbu's method, specifically for solutions which are L^∞ or bounded. Such solutions arise frequently in kinetic theory and are of greater practical interest than L^1 solutions.

Corollary 3.1. *If the space homogeneous Boltzmann equation has a non-negative solution $f \in L^\infty$, then the solution $\tilde{f}$ of the DMC-KDE method converges strongly in L^∞ to f. That is*

$$\lim_{\Delta t \to 0} \lim_{N_p \to \infty} \|\tilde{f} - f\|_\infty = 0.$$

Proof. Take any $\epsilon > 0$. Since $\tilde{f}, f \in L^\infty$, there exist $B_1, B_2 \in \mathbb{R}^+$ such that $|\tilde{f}(\vec{x})| \leq B_1$ and $|f(\vec{x})| \leq B_2$ almost everywhere. Let S_1 and S_2 be the sets of zero measure over which these inequalities do not hold for $\tilde{f}$ and f respectively. Let $S = S_1 \cup S_2$. For any $\vec{x'} \in \mathbb{R}^3 - S$, define

$$\phi_h(\vec{x}) = \frac{1}{\sqrt{2\pi}h^3} \exp\Big(- \frac{\|\vec{x} - \vec{x'}\|^2}{h^2} \Big).$$

By Lemma 3.1, ϕ_h is a delta family as $h \to 0$ centered at $\vec{x'}$. Therefore, there exists $H > 0$ such that

$$\Big| \int_{\mathbb{R}^3} \phi_h(\vec{x})(\tilde{f}(\vec{x}) - f(\vec{x}))dx - (\tilde{f}(\vec{x'}) - f(\vec{x'})) \Big| < \frac{\epsilon}{2},$$

for all $h < H$. Thus,

$$|\tilde{f}(\vec{x'}) - f(\vec{x'})| < \frac{\epsilon}{2} + \Big| \int_{\mathbb{R}^3} \phi_h(\vec{x})(\tilde{f}(\vec{x}) - f(\vec{x}))dx \Big|.$$

Note that ϕ_h is everywhere continuous and

$$|\phi_h(\vec{x})| \leq \frac{1}{\sqrt{2\pi}h^3},$$

for all $\vec{x} \in \mathbb{R}^3$. Thus by Theorem 3.2, there exist $N > 0$, $d > 0$ such that

$$\Big| \int_{\mathbb{R}^3} \phi_h(\vec{x})(\tilde{f}(\vec{x}) - f(\vec{x}))dx \Big| < \frac{\epsilon}{2},$$

for all $N_p > N$, $\Delta t < d$. Therefore from Eq. (3.2), we have

$$\begin{aligned} \|\tilde{f} - f\|_\infty = & \operatorname{ess\,sup} |\tilde{f} - f| = \sup_{\vec{x'} \in \mathbb{R}^3 - S} |\tilde{f}(\vec{x'}) - f(\vec{x'})| \\ < & \frac{\epsilon}{2} + \int_{\mathbb{R}^3} \phi_h(\vec{x}) |\tilde{f}(\vec{x}) - f(\vec{x})| dx \\ < & \frac{\epsilon}{2} + \frac{\epsilon}{2} = \epsilon. \end{aligned}$$

So, the proof is completed. □

Corollary 3.2. *If the space homogeneous Boltzmann equation has a non-negative bounded solution f, then the solution $\tilde{f}$ of the DMC-KDE method converges pointwise to f.*

Proof. The proof follows naturally from Corollary 3.1. □

3.3 Numerical implementation

To demonstrate the DMC-KDE method numerically, we modeled the relaxation of a space homogeneous gas in the absence of external forces from a uniform initial velocity distribution. The initial condition for the test case is given by

$$f(\vec{c},0) = h(c_x)h(c_y)h(c_z), \tag{3.14}$$

where

$$h(x) = \begin{cases} \dfrac{1}{2}, & \text{if } |x| \leq 1, \\ 0, & \text{if } |x| > 1. \end{cases}$$

Knowing that the steady state solution in this case must be of Maxwellian form, one may determine that the steady state solution is given by

$$f_\infty(\vec{c}) = \Big(\frac{3}{2\pi}\Big)^{\frac{3}{2}} \exp\Big(-\frac{3\|\vec{c}\|_2^2}{2}\Big). \tag{3.15}$$

The evolution of the x-component velocity distribution is shown in Fig. 1. These results were obtained using only twenty simulated particles and averaged over an ensemble of one-thousand simulations. In order to obtain an understanding of the convergence of the method, 100 runs were performed for 5 different values of N_p and the cumulative error was computed at $t = 0.15$ a condition nearing steady state. The results are shown in Fig. 2. Note that as previously shown, the Nanbu approach does not converge in this sense, whereas convergence is apparent in the DMC-KDE results.

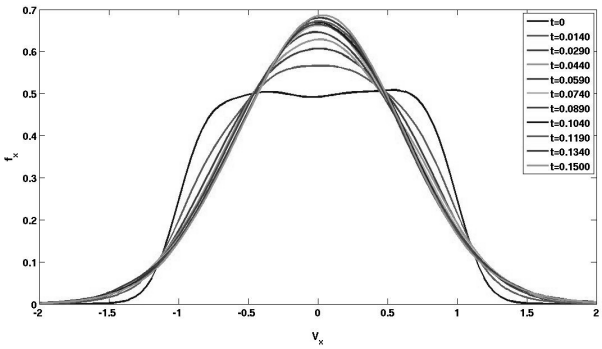

Figure 1: DMC-KDE Solution of Test Case. $N_p = 20$, $N_{samp} = 1000$.

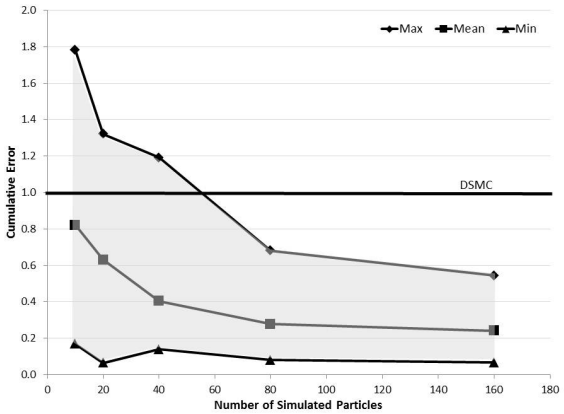

Figure 2: Cumulative Error for 100 runs of DMC-KDE Method.

Although having relaxed some of the assumptions inherent to DSMC, the DMC-KDE has inherent assumptions of its own. First, the particle densities are constrained to be Maxwellian throughout the entire simulation. Secondly, the collision selection criteria are consistent only in the limit as N_p becomes large. Finally, because of the constraint that distributions must be Maxwellian, collision modeling cannot take full advantage of the distributional framework. Ideally, a fully distributional method would relax each of these constraints: allowing for generalized particle distributions, providing for consistent collision selection criteria, and treating collision interactions as relaxation processes of the collections of actual particles involved. Nevertheless, the DMC-KDE approach represents a new stochastic Boltzmann solver which although possessing many similarities to DSMC achieves convergence properties that are not obtainable with DSMC.

4 A simplified distributional Monte Carlo approach using the BGK equation

We seek to develop a fully distributional method, with collision selection criteria and modeling that fully incorporates generalized particle velocity distributions. The analysis is much more complicated when generalized velocity distributions are involved, so as a proof of concept case, a simplified scheme was developed. In this case, collision selections are performed based upon the DMC-KDE criteria using the mean particle velocity. The collision modeling however is modified to take advantage of the distributed particle velocities, and the particle velocity distributions themselves are now estimated using kernel density estimation.

The collision modeling step utilizes the Bhatnagar-Gross-Krook (BGK) equation [7] to evolve the joint velocity distribution of the two particles in a collision pair. Although not fully consistent with the Boltzmann equation, the BGK model has been employed in various forms to many applications in rarefied gas dynamics [12, 15, 25]

and thus serves as a suitable starting point for our efforts. The BGK equation replaces the complex collision integral of the Boltzmann equation with a simplified model as follows.

$$\begin{aligned}&\frac{\partial}{\partial t}f(\vec{r},\vec{c},t)+\vec{c}\cdot\frac{\partial}{\partial \vec{r}}f(\vec{r},\vec{c},t)+\vec{F}\cdot\frac{\partial}{\partial \vec{c}}f(\vec{r},\vec{c},t)\\ =&\nu(f(\vec{r},\vec{c},t)-f_\infty(\vec{r},\vec{c})),\end{aligned}\tag{4.1}$$

where ν is collision frequency and f_∞ the steady state solution (typically Maxwellian) that the gas is assumed to be relaxing towards. Although the BGK equation can not be directly extracted from the Boltzmann equation, the model tends to capture many of the relevant features exhibited by it especially when ν is allowed to vary with molecular velocity. Other, more complex BGK models (e.g., Ellipsoidal Statistical Model) exist and have been shown to provide solutions which are more physically meaningful than the basic BGK model [10]. In the space homogeneous case with no external forcing, the BGK equation reduces to a first order ordinary differential equation

$$\frac{\partial f}{\partial t}(\vec{c},t)=\nu(f(\vec{c},t)-f_\infty(\vec{c})).\tag{4.2}$$

Assuming a constant collision rate, the solution of Eq. (4.2) is given by

$$f(\vec{c},t)=e^{-\nu t}f_0(\vec{c})+(1-e^{-\nu t})f_\infty(\vec{c}).\tag{4.3}$$

We will employ Eq. (4.3) to evolve the combined probability distribution function of two simulated particles in a collision interaction.

To facilitate this, we begin by generalizing the method to allow for non-Gaussian distributions on each simulated particles velocity distribution function. To achieve this and allow greater flexibility, the distributed particle velocities are estimated using KDE at the particle level instead of at the overall distributional level. The overall distribution is given by

$$\hat{f}=\frac{1}{N_p}\sum_{i=1}^{N_p}f_i.$$

The f_i is the i^{th} simulated particle's velocity distribution given by

$$f_i(\vec{c})=\frac{1}{N_v h^3}\sum_{j=1}^{N_v}K\Big(\frac{\vec{c}-\vec{c_{ij}}}{h}\Big),$$

where N_v is the number of velocity samples in the kernel density estimate of each particle's velocity distribution function, $\vec{c_{ij}}$ is the j^{th} velocity sample of the i^{th} particle's distribution function, and h is now given by

$$h=\Big[\frac{32}{3\sqrt{2}N_pN_v}\Big]^{\frac{1}{5}}\sigma_{est}.$$

As mentioned previously, the collision modeling step is performed by evolving the combined distribution function of the collision pair through Δt using the BGK equation. N_v velocities are then re-sampled from the resulting distribution for each particle to determine new particle distribution functions. The solution to the BGK equation remains as in Eq. (4.3), however, the initial and final distributions are now based upon only the two particle distributions involved in the collision. For a collision pair (i,j),

$$f_0(\vec{c}) = \frac{1}{2}(f_i(\vec{c}) + f_j(\vec{c})), \qquad f_\infty(\vec{c}) = \frac{1}{\pi^{\frac{3}{2}}\tilde{h}^3}\exp\Big(-\frac{\|\vec{c}-\tilde{c}\|^2}{\tilde{h}^2}\Big),$$

$$\nu \approx \frac{2N}{N_p\Delta t}, \qquad \tilde{c} = \frac{1}{2N_v}\sum_{k=1}^{N_v}(\vec{c}_{ik}+\vec{c}_{jk}),$$

$$\tilde{h} = \sqrt{h^2 + \Big(\sum_{k=1}^{N_v}\|\vec{c}_{ik}\|^2 + \|\vec{c}_{jk}\|^2\Big) - \frac{2}{3}\|\tilde{c}\|^2}.$$

To demonstrate the potential benefits of such a scheme, we simulated the same problem discussed in Section 5. The results of the Simplified DMC method are shown in Fig. 3. These results show drastic improvement over the DMC-KDE results with a

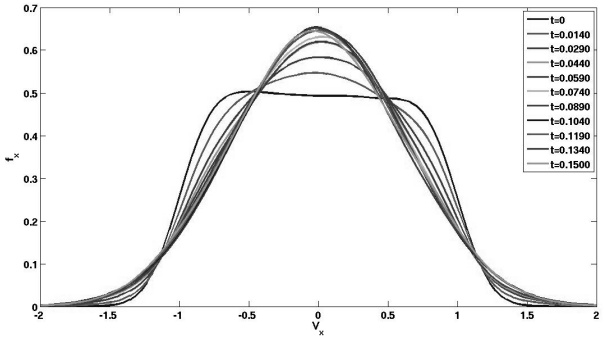

Figure 3: Simplified DMC Solution of Test Case. $N_p = 20$, $N_{samp} = 16$, $N_v = 20$.

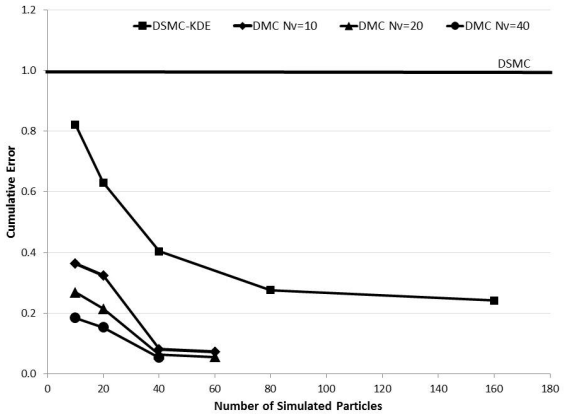

Figure 4: Mean Cumulative Error for 100 runs of Simplified DMC Method.

significantly reduced value of N_p.

In order to obtain an understanding of the convergence of the method, 100 runs were performed for 5 different values of N_p and 3 different values of N_v. The cumulative error was computed was computed at $t = 0.15$. The results for the mean cumulative error are shown in Fig. 4 as they vary with N_p and N_v. Marked improvement has been achieved in terms of reduction in the cumulative error. It should be noted that the computational demands of including an additional velocity sample per particle (increasing N_v) are lower than those for including an additional simulated particle (increasing N_p). Considering the results shown in Fig. 4, it seems reasonable that more samples per particle may be desirable for improving accuracy at lower values of N_p, whereas at higher values of N_p, the effect is diminished. It would seem that N_p remains the primary driver of accuracy.

5 Conclusions

We have presented a distributional Monte Carlo approach which employs results from kernel density estimation to provide convergence in solution, rather than only convergence in probability measure (as in the case of DSMC). Specifically, we have proven that the DMC-KDE scheme maintains convergence in probability measure (weak convergence) for L^1 space homogeneous solutions, while obtaining strong convergence for L^∞ and bounded solutions. In this sense, the DMC-KDE approach would be considered a stochastic Boltzmann solver, rather than a simulation process. To our best knowledge no formal proofs of the type of convergence we have exhibited appear in the literature for existing Monte Carlo approaches for the Boltzmann equation.

The DMC-KDE approach achieves this convergence by relaxing some of the assumptions inherent to DSMC. Specifically, instead of assuming that each of the actual particles represented by a simulated particle all possess the same velocity, it is assumed that the collections actual molecular velocities are distributed according to a Maxwellian (equilibrium) distribution. This assumption itself imposes a constraint on the method, namely that non-Maxwellian particle distributions are not provided for. Nevertheless DMC-KDE serves as a first step toward a fully distributional approach which would allow generalized particle distributions and compute collision interactions as relaxation process over the collection of actual molecules represented by the simulated particles undergoing a collision. We have presented our initial findings in our development of a DMC scheme with collision modeling based upon the BGK equation which has been employed in various forms to many applications in rarefied gas dynamics. The numerical results we have presented show significant improvement over DMC-KDE for the example problem we considered. Our initial results suggest that the increased computational cost associated with this new framework are not prohibitive, and the effect of distributing the particle velocities has significant impact on the accuracy of the solution.

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