Distributional Collision Modeling for Monte Carlo Simulations

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Abstract. In this paper we present the initial results in our development of Distributional DSMC (DDSMC) methods. By modifying Nanbu's method to allow distributed velocities, we have shown that DSMC methods are not limited to convergence in probability measure alone, but can achieve strong convergence for L^1 solutions of the Boltzmann equation and pointwise convergence for bounded solutions. We also present an initial attempt at a general distributional method and apply these methods to the Bobylev, Krook, and Wu space homogeneous solution of the Boltzmann equation.

Keywords: DSMC, Boltzmann Equation, Kernel Density Estimation
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INTRODUCTION

The Direct Simulation Monte Carlo (DSMC) method represents a probabilistic simulation of the interactions of a fraction of the number of actual particles in a gas. An important parameter in such simulations is the statistical particle weight $W = N/N_p$ which represents the total number of actual particles that each simulated particle represents. In practice, W may be on the order of 10^6 or greater. In traditional DSMC methods, particles may possess only a single velocity, energy state, and position at any point in the simulation. This gives rise to a singular or discrete probability density function

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

Nanbu [1] developed an approximation to the solution of the space homogeneous Boltmann equation with the above expression as the initial condition. Utilizing this solution, Nanbu developed a DSMC scheme. Babovsky and Illner later proved that Nanbu's scheme converged in probability measure to the solution of the Boltzmann equation [2, 3].

Although mathematically convenient, the representation of the distribution function in Equation (1) is nonphysical in any case where $N_p < N$. The assumption of singular velocities has significant implications on the results obtained by such a scheme. Specifically, we suggest that this assumption is responsible for a significant portion of the variance associated with DSMC methods. This is evident when one considers the implications for the evolution of the velocity distribution function. When two simulated particles have their velocities altered by a collision, we presume that the millions of acutal particles these particles represent all depart on the same velocity vector, resulting in a significant change to the distribution function. In reality, these millions of particles cannot possess the same exact velocity, and the collision interaction is more aptly described as an evolution of the distribution function by collisional effects.

From this premise, we have undertaken a study to explore the value and complications of incorporating distributed particle velocities in the DSMC framework [4, 5]. We propose that if a scheme can be developed which allows a particle's velocity to be distributed, improved convergence and variance reduction should be achievable.

Toward this end, we have developed two methods for attempting to distribute a particle's velocity. The first, applies kernel density estimation (KDE) to the DSMC method and allows each particle's velocity to be distributed according to a Gaussian. The second, more general method we have developed is termed Distributional DSMC. In this construct, kernel density estimation methods are applied at the particle level to allow each particle's velocity to be distributed arbitrarily.

DSMC-KDE

As we have already presented results relating to the development of the DSMC-KDE method [4, 5], we present only a brief overview of the key features here. The basic premise relies on the replacement of the distribution function described by Equation (1) with the following kernel density estimator

$$\tilde{f}(\vec{c}) = \frac{1}{N_p h^3} \sum_{i=1}^{N_p} K\left(\frac{\vec{c}-\vec{c}_i}{h}\right) \tag{2}$$

Here K is the kernel function, which we choose to be a Gaussian. Namely,

$$K(\vec{x}) = (2\pi)^{-3/2} \exp\left(-\frac{\|\vec{x}\|^2}{2}\right) \tag{3}$$

h is termed the collision bandwidth, and should be chosen in such a way as to minimize the error between the actual distribution and the estimator. Based on the results of Wand & Jones [6] we choose h as follows

$$h = \left[\frac{32}{3\sqrt{2}N_p}\right]^{\frac{1}{5}} \hat{\sigma} \tag{4}$$

Where $\hat{\sigma}$ is an estimate of the standard deviation of f. The key feature here is that h is choosen to depend on N_p in such a way that $\lim_{N_p\to\infty} h(N_p) = 0$. It can be shown that K becomes a delta family as $N_p \to \infty$.

We have shown [4] that this interpretation results in identical collision selection and modeling rules for the center points of the Maxwellians in the limit as $N_p \to \infty$ and that the stochastic rules governing the evolution of the simulation can be chosen to be identical to Nanbu's method. Equivalently, Equation (2) may simply be interpreted as a kernel density estimator which utilizes the particle velocities obtained via Nanbu's method as samples of the overall distribution function. In this case, the stochastic simulation remains the same as Nanbu's method and the distribution function may be calculated from Equation (2) post-simulation. It should be noted that Nanbu's model was selected for this effort because of its traceability to the Boltzmann equation but it is not necessarily the most desirable model for implementing this method for practical applications. Rather, we utilize Nanbu's method to identify the potential benefits of the Distributional DSMC Concept which should be applicable to any existing method.

Utilizing this interpretation, we have proven [4] that this method maintains the convergence demonstrated for existing methods, achieves strong convergence for L^∞, and pointwise convergence bounded solutions, niether of which is possible with the original method. Such solutions arise frequently and are of greater practical interest than the general L^1 case. As the main thrust of this paper is not a detailed mathematical proof of convergence, these results are summarized here in the following theorems.

Theorem 1. *If the Boltzmann equation with initial data f_0 has a non-negative solution $f \in L^1$, then the solution $\tilde{f}$ of the DSMC-KDE method converges weakly in L^1 to f such that for any bounded and continuous test function ϕ on $\mathbb{R}^3$,*

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

Corollary 1. *If the Boltzmann equation with initial data f_0 has a non-negative solution $f \in L^\infty$, then the solution $\tilde{f}$ of the DSMC-KDE method converges strongly in L^∞ to f. That is,*

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

Corollary 2. *If the Boltzmann equation with initial data f_0 has a non-negative bounded solution f, then the solution $\tilde{f}$ of the DSMC-KDE method converges pointwise to f.*

The DSMC-KDE method was developed to serve as a stepping stone and building block of a more comprehensive method. Although not a fully distributional method, we have shown [4, 5] that stronger forms of convergence than acheivable by traditional DSMC are possible.

DISTRIBUTIONAL DSMC

We next sought to develop a fully distributional method, which would allow for particle velocities to be distributed arbitrarily. Development of a fully distributional method requires a full re-derivation of the DSMC algorithm. We have developed a simplified scheme that allows reuse of the existing collision selection rules while modelling intermolecular collisions in a fully distributional sense.

The basic premise is to apply kernel density estimation at the particle level distribution functions instead of at the overall distribution function level. This allows a particle's velocity to be distributed arbitrarily, limited only by the number of velocity samples per particle, N_v. In this case, the i^{th} particle's distribution function is given by

$$f_i(\vec{c}) = \frac{1}{N_v h^3} \sum_{j=1}^{N_v} K\left(\frac{\vec{c} - \vec{c}_{ij}}{h}\right) \tag{5}$$

where $\vec{c}_{ij}$ is the j^{th} velocity sample in the i^{th} particle's distribution, K is given by Equation (3) and h is now given by

$$h = \left[\frac{32}{3\sqrt{2}N_p N_v}\right]^{\frac{1}{5}} \hat{\sigma} \tag{6}$$

The overall distribution function may therefore be written as

$$\tilde{f}(\vec{c}) = \frac{1}{N_p N_v h^3} \sum_{=1}^{N_v} K\left(\frac{\vec{c} - \vec{c}_{ij}}{h}\right) \tag{7}$$

Developing a collision selection criteria based on Equation (7) is a non-trivial excercise. To simplify the process, we assume (only for the purpose of collision selection) that a particle's velocity distribution is in some sense "close" to a Gaussian centered at its mean velocity. Under this assumption, the selection criteria can be chosen to be the same as Nanbu's method (or the DSMC-KDE method) based upon the mean particle velocities.

Once a collision pair has been identified, we seek to evolve the combined velocity distribution of the pair through the time step Δt. The combined distribution of a collision pair is given by

$$F(\vec{c}) = \frac{1}{2}\left[f_i(\vec{c}) + f_j(\vec{c})\right] = \frac{1}{2N_v h^3} \sum_{k=1}^{N_v} K\left(\frac{\vec{c} - \vec{c}_{ik}}{h}\right) + K\left(\frac{\vec{c} - \vec{c}_{jk}}{h}\right) \tag{8}$$

The process by which the combined distribution is evolved through Δt is a topic to be explored in future work. Conceptually, any method which is consistent with the Boltzmann equation should be useable. Such a method might be a moment method, model equation, or even DSMC itself. For our initial development we utilized the BGK equation, however as the BGK equation is not consistent with the Boltzmann equation we utilized this model only for testing purposes. The method we have currently implemented employs DSMC-KDE to evolve the combined distribution function. In the limit as N_v becomes large, the method becomes fully consistent with the DSMC-KDE model with $2N_v$ simulated particles, and the method may be reapplied to compute interactions between these samples. This has an interesting side effect in that it allows any particle which is selected for collision to self interact. This would be impossible if each simulated particle represented one actual particle, but as each simulated particle represents a large collection of particles this is perfectly acceptable, and in fact desirable.

NUMERICAL IMPLEMENTATION

To explore the DDSMC method currently proposed we applied the scheme to the space homogeneous solution of Bobolev, Krook, and Wu [7]. To further simplify, we assume the Maxwellian molecular model. The distribution function is spherically symmetric and in this case the distribution of molecular speed is given by [1]

$$F(c,\tau) = 4\pi(\pi\alpha)^{-\frac{3}{2}}\left(\alpha_1\hat{c}^2 + \alpha_2\hat{c}^4\right)\exp\left(-\frac{\hat{c}^2}{\alpha}\right) \tag{9}$$

where,

$$\begin{aligned}
\alpha_1 &= \frac{5\alpha - 3}{2\alpha} \\
\alpha_2 &= \frac{1-\alpha}{\alpha^2} \\
\hat{c} &= \frac{c}{\sqrt{2kT/m}} \\
\alpha(\tau) &= 1 - \frac{2}{5}e^{-\tau} \\
\tau &= \pi A_2(5)\, nt\sqrt{2b/m}
\end{aligned}$$

The results of this analysis are shown in Figure 1. Figure 2 shows the mean steady state L^1 error for a 100 run

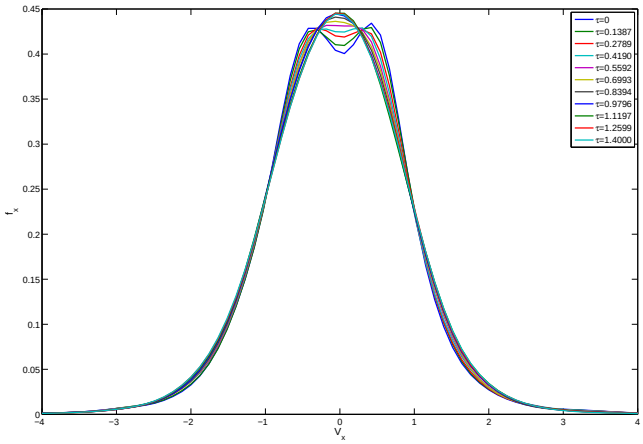

FIGURE 1. DDSMC Solution for x-velocity Distribution of the Krook-Wu Problem. $N_p = 20$, $N_v = 16$, $N_{samp} = 100$, $\Delta\tau = 1.4E-3$, Total Computational Time = 46.27 sec

ensemble as a function of N_p and N_v. Here we see significantly improved results over the original Nanbu method, as well as DSMC-KDE. Finally in Figure 3 we have the computational time per sample as a function of N_p and N_v. Note that although the computational time per sample is increased by the additional complexity of the method, the increase in accuracy over the DSMC-KDE method far outweighs the drawbacks. This is evident in Figures 4 and 5 where the values are plotted against the total number of parameters per sample, N_pN_v.

CONCLUSIONS AND FUTURE WORK

Our current results would seem to indicate that there is potentially significant benefits to be gained by distributing particle velocities in DSMC simulations. Future work will focus on formally analyzing the convergence and computational complexity of the Distributional DSMC method. Although the current work is limited to the space homogenous case, it is conjectured that the method should be fairly easily generalized to multiple dimensions. The variance reduction properties of these methods are yet to be addressed, however, we believe significant benefits may be otained. The effect of a particle carrying its distribution function through the flowfield may have a similar effect as Information Preservation DSMC.

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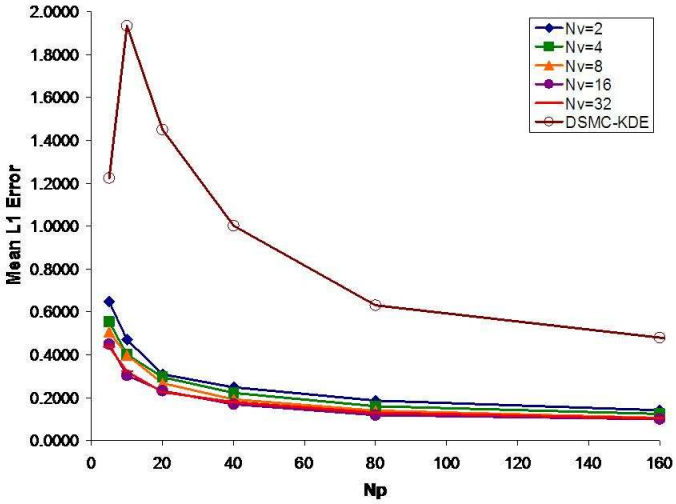

FIGURE 2. Steady State L^1 Error for 100 Run Ensemble as a Function of N_p

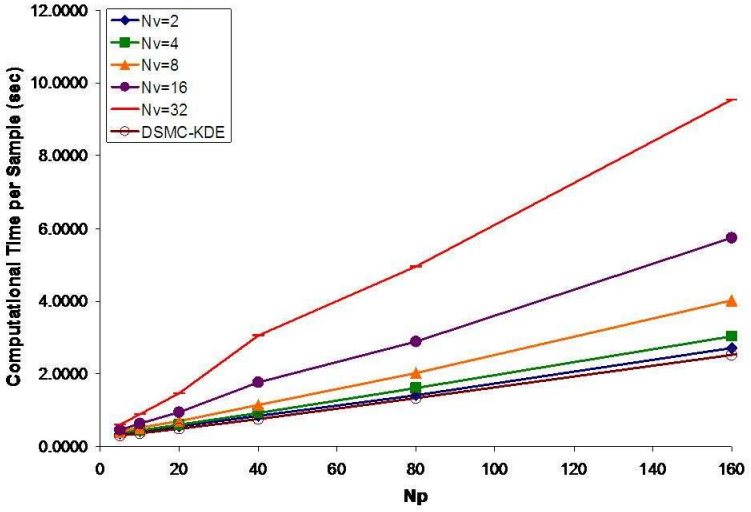

FIGURE 3. Computational Time per Sample as a Function of N_p

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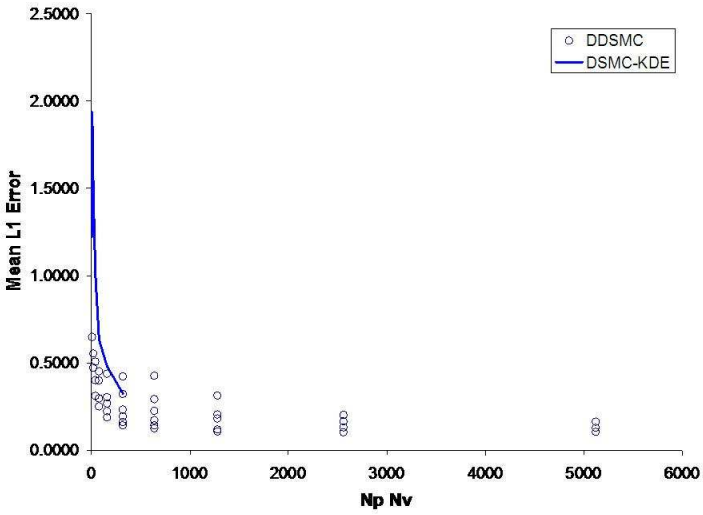

FIGURE 4. L^1 Error for 100 Run Ensemble as a Function of N_p

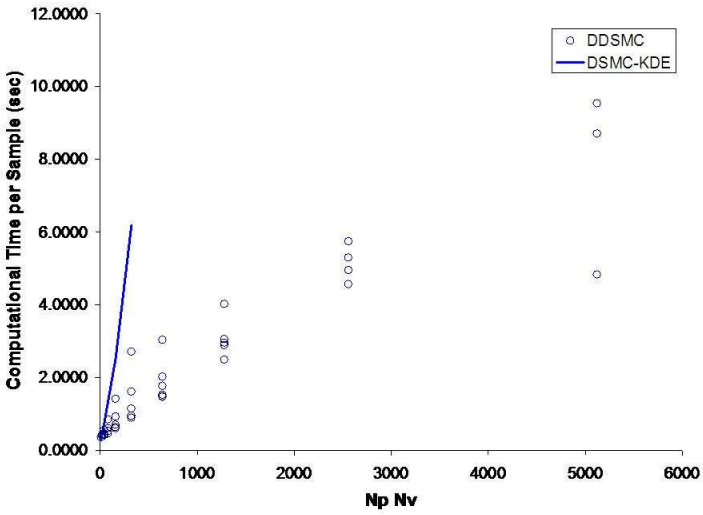

FIGURE 5. Computational Time per Sample versus Total Number of Parameters